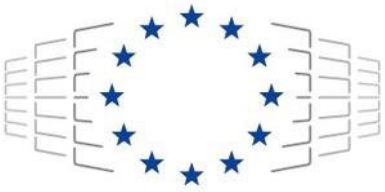
HORIZON-EUROHPC-JU-2021-COE-01

The European Centre of Excellence for Engineering Applications

Project Number: 101092621

D5.1
Services, Training and Portal Progress Report



The EXCELLERAT P2 project has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 101092621. The JU receives support from the European Union's Horizon Europe research and innovation programme and Germany, Italy, Slovenia, Spain, Sweden and France.

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Dissemination Level	Public	

Date	Author	Comments	Version	Status
2023-10-13	All	Initial draft	V0.1	Draft
2023-10-24	All	All available content merged	V0.2	Draft
2023-10-25	All	All available content merged	V0.3	Draft
2023-10-25	TCM	Adding section 2 Service Provisioning	V0.4	Draft
2023-10-25	All	All available content merged	V0.5	Draft
2023-10-26	All	Completed chapter 5, conclusions, references	V0.6	Draft
2023-10-26	All	All available content merged	V1.0	Ready for review
2023-11-03	CA	Addressed comments	V2.0	Pre-final
2023-11-06	TZ	Addressed comments in Section 4	V2.1	Pre-final
2023-11-08	MD	Addressed comments in Section 3	V2.3	Pre-final
2023-11-08	FG	Minor corrections in Section 2	V2.4	Pre-final
2023-11-22	All	ABB 2nd review comments addressed	V3.1	Pre-final
2023-12-13	CA	MM 2nd review comments addressed	V3.2	Pre-final

List of abbreviations

AI	Artificial Intelligence
API	Application Programming Interface
CFD	Computational Fluid Dynamics
CoE	Centre of Excellence
CPU	Central Processing Unit
DAT	Data in HPC
DEM	Discrete Element Method
DL	Deep Learning
ESP	EXCELLERAT Service Portal
EU	European Union
FEM	Finite Element Method
FhG	Fraunhofer Gesellschaft
FPGA	Field Programmable Gate Array
GPU	Graphics Processing Unit
HPC	High-Performance Computing
ICT	Information and Communication Technology
IR	Infra-red
ISV	Independent Software Vendor
ITER	International Thermonuclear Experimental Reactor
JU	Joint Undertaking
KPI	Key Performance Indicator
ML	Machine Learning
NCC	National Competence Centre
PAR	Parallel Programming
PMT	Project Management Team
RQL	Rich-Burn, Quick-Mix, Lean-Burn
SME	Small and Medium Enterprise
UL	University of Ljubljana
UX	User experience
VIS	Scientific Visualisation
WEST	Tungsten (W) Environment in Steady-state Tokamak
WP	Work Package
Y	Year

Executive Summary

This deliverable D5.1 "*Services, Training and Portal Progress Report*" presents the outcomes of the first year of Work Package (WP) 5 activities for all its four tasks.

Task 5.1 *Service Provisioning*: the new EXCELLERAT Service Portal graphic design has been developed according to the result of the satisfaction survey of the users.

Task 5.2 *Training and Education*: four main training events have taken place during the first 10 months of the project. Overall, the training event contents and lectures received positive feedback from the participants.

Task 5.3 *Resource Acquisition*: as the EuroHPC JU has not yet defined a special access scheme to computational resources for Centres of Excellence, the activity of task 5.3 for the first year consisted mainly of collecting information in collaboration with CASTIEL 2. The computational requirements of the various EXCELLERAT P2 use cases were estimated, and input from the code owners concerning the service offerings were collected.

Task 5.4 *Further Applications*: The application form for the onboarding of new applications through the service portal is currently being developed. In the meantime, task 5.4 has been collaborating with the technical WPs in following the first onboarded use case, the digital twin of the first wall of a tokamak fusion reactor, which is currently proceeding on schedule. Additionally, an onboarding request from DCS Computing GmbH forwarded by the Austrian NCC is being evaluated.

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1 Introduction

This document summaries the work performed in work package 5 from the beginning of the project to the end of the first year. It also contains an outlook on the development of the services provided by the centre, the concepts and experiences with the operation and implementation of services and training. Before analysing the progress of the tasks embodied in WP5, we introduce the main role and a description of this work package.

Work package 5 was designed to fulfil three main purposes, related to the management of services and training:

- To manage the services offered by EXCELLERAT P2, in particular to support the implementation of the services for external users. These services fulfil the requirements defined in the technical work packages WP1, WP2 and WP4 and are in line with the business model presented in WP6. A service portal was developed during phase 1 of EXCELLERAT. One of the tasks of WP5 is therefore to redesign the service portal to improve the technical aspects and user experience and to incorporate the new services introduced in the second phase of the project.
- To structure training modules about the project results and to cover the gaps identified in the EU market relative to the addressed topics. Again, the previous mentioned Service Portal turns out to be a fundamental tool for dissemination: the portal provides an access point for training and for searching for use cases. The new version under development will be fully aligned with the EuroCC Access and the C2ICCS portals and will allow the exchange of information on new trainings and events through APIs, allowing a wider distribution to public, especially to other CoEs and EuroCC National Competence Centres (NCCs) partners.
- To support partners in the acquisition process of computational resources needed to achieve the goals listed in the technical work packages, e.g. by responding to EuroHPC open calls.

To achieve the previous objectives, WP5 is structured in four tasks, which will be briefly summarised below.

Task 5.1: Service Provisioning. This task involves the Service Portal maintenance and enhancement. As mentioned, the Service Portal provides access to the EXCELLERAT services, which allows to search for use cases and facilitates the dissemination process. This task sees the collaboration of all partners, especially for the implementation of new services, among these, we mention:

- Co-design and solution consulting.
- Code porting, benchmarking, optimisation consulting.
- Scalable visualisation workflows and interactive tools deployment.
- Data-analytics business logic implementation.
- Best practices/use cases implementation guidelines.
- Providing easy access to Data Exchange with HPC for processing data.
- Full-Service Data Workflow Management for scientific data calculation.
- Very high automation with AI attempts for dispatching scientific data to HPC codes.

By the end of the first year, a comprehensive update of the previous version of the portal is expected, with added new services.

Task 5.2: Training and Education. This task is devoted to training and education, and it is structured in the following points, built on the outcomes of EXCELLERAT P1:

- Exploit and updating the training activities already offered by the consortium members.
- Realise new initiatives to extend the existing offer developed during EXELLERAT P1, i.e. the training material on scientific visualisation with COVISE and VISTLE, two software environments for simulation and visualisation.
- Expand the collaboration with the NCCs established by the project EuroCC and with other EuroHPC initiatives such as EuMaster4HPC, an HPC European consortium by implementing the first pan-European HPC Master programme.
- During the first phase of EXCELLERAT training models about data analytics for simulations have been developed by our partner Fraunhofer Gesellschaft (FhG), the aim is to adapt them to new developments and to provide additional workshops, again with the support of FhG. These training modules will be offered as open or in-house training courses by the CoE.

Task 5.3: Resource Acquisition. This task provides a link between the CoE and the European HPC infrastructures in order to guarantee the HPC resources needed for the accomplishment of the other work packages. Hence this task includes:

- Allocation of CPU time, debugging activities and CoE experiments.
- User support on HPC systems.

Task 5.4: Further Application. This task covers many aspects to guarantee a continuity to the project.

- It ensures that new EXCELLERAT users are integrated into established procedures, including requirements assessment and application development.
- It collaborates with task 7.2 to reach out to the community codes, i.e. to bring in technical expertise related to community codes that are not yet part of EXCELLERAT's technical WPs.
- The first use case concerns the setup of a digital twin of the first wall of a tokamak fusion reactor to contribute to the optimisation of this crucial component of a tokamak fusion reactor by better explaining the physical processes around the inner wall during the fusion reactions.
- Monitoring the development of large use cases.

From the previous list, it is evident that WP5 acts in close in cooperation with other WPs, especially the technical work packages WP2, WP3 and WP4. To better visualise its role, it is possible to consult the work packages organisation in Figure 1. In particular, the technical work packages are responsible for defining and validating services that will be approved by WP1 with the collaboration of WP6 to accommodate them into the CoE business model, that will be implemented by WP5. WP5, in turn, will manage the requests for onboarding new use cases, that will be approved by WP1 and the technical work packages. Their execution and monitoring will then fall under WP2.

Having described the tasks and purposes of WP5, we now proceed to analyse the progress of each of these tasks. In the following, each section is dedicated to one of the tasks described above. In particular, Section 2 deals with Task 5.1 – *Service Provisioning*, which describes the Service Portal and its redesign compared to the previous version. Section 3 deals with Task 5.2 - *Training and Education*. This section lists the EXCELLERAT P2 training events and analyses the corresponding KPIs; at the end of the section, an outlook on the future roadmap is given. Section 4 is dedicated to Task 5.3 – *Resource Acquisition*. The first part of the section describes the access scheme to the EuroHPC JU systems; the second part presents the results of the survey on users' experiences and expectations regarding access to computing resources. Finally, in Section 5, Task 5.4 - *Further applications* is addressed, where a full description of the service portal workflow for an onboarding procedure can be found, the onboarding application under

review, and in the last part, a description and progress of the use case related to the digital twin of the tokamak. In the conclusion section, we summarise our main findings and progress.

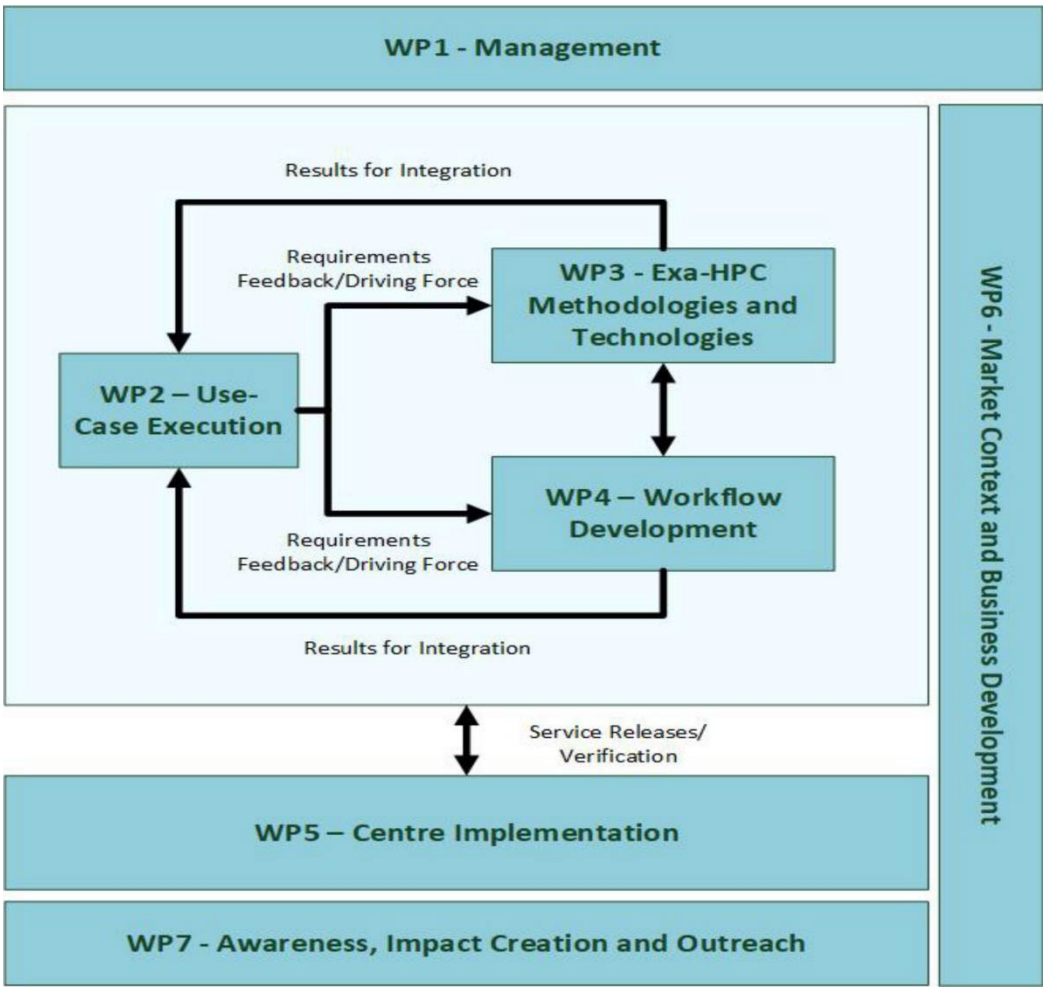

Figure 1: Relations between WP5 and the other WPs

2 Service provisioning

2.1 EXCELLERAT Service Portal Introduction

The EXCELLERAT Service Portal (ESP) [1] was developed during the first project phase. ESP serve as a first contact point between the users and the EXCELLERAT members, who are offering services. The portal is working as a catalogue, listing and presenting services, which could be requested by users. Users can search for services through three dashboards: Community, Engineer and Developer.

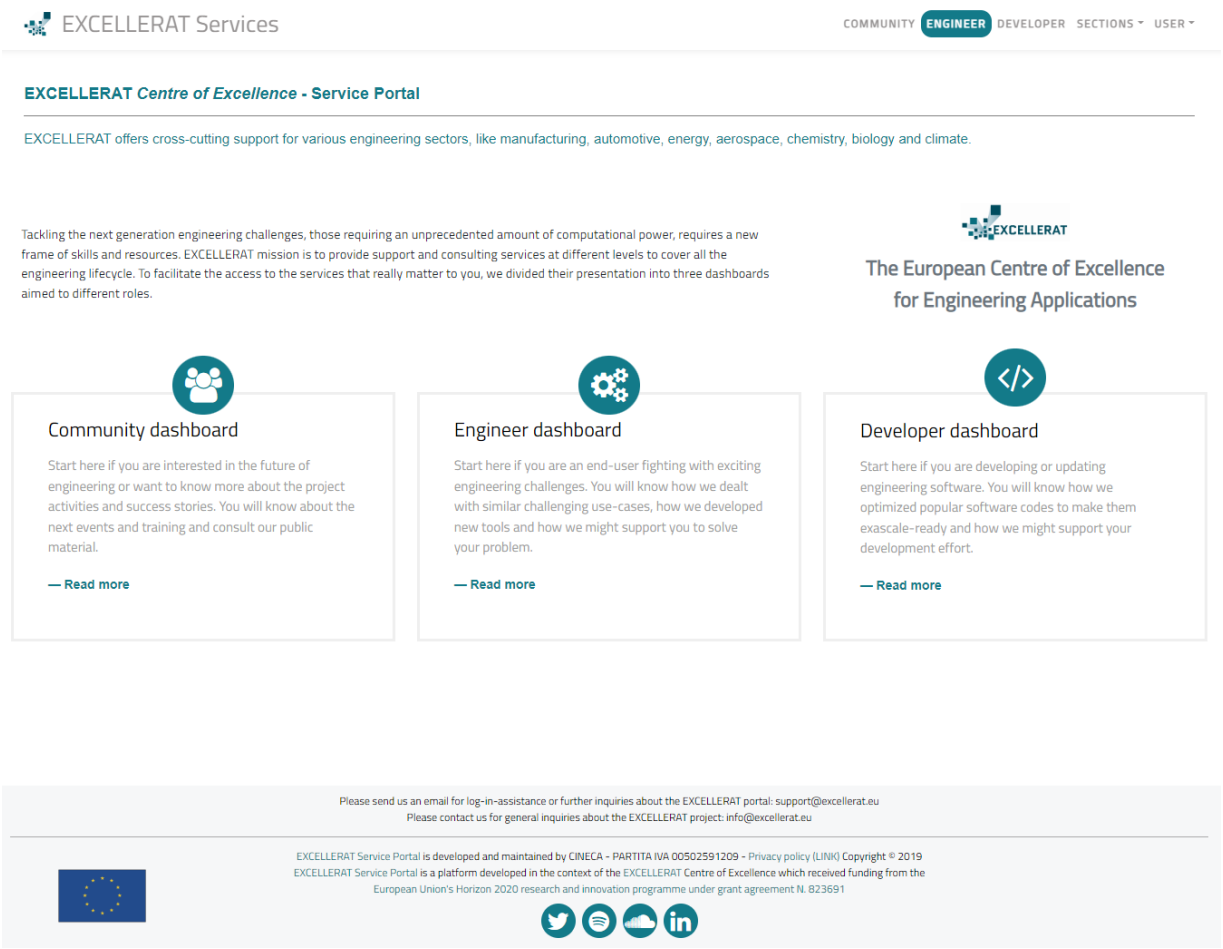

Figure 2: EXCELLERAT Service Portal Landing Page

2.2 EXCELLERAT Service Portal Redesign

During the first phase of the project, the partners have already collected user feedback on the use of the ESP. In order to provide users with the best possible user experience, the improvement of the ESP was planned for the second phase of the project. As part of WP5 and in collaboration with WP6 and WP7, it is planned to significantly improve the platform both technically and in terms of design and user-friendliness. To achieve this goal, the following activities were planned and carried out (M1-M9):

- Definition of methodologies, standards and technical implementation.
- Analysis of the ESP.
- Acquisition of internal and external user feedback, performing of user interviews.
- Analysis of user feedback and information.

- Analysis of user experience and ESP improvement, with further recommendations derived.
- Discussion and development of specifications for ESP redesign and further maintenance.
- Discussion of a portal technical implementation within the CI2SS Portal (CASTIEL 2 [2]) discussed, with further inputs provided to the CASTIEL 2 Team.
- Development of an ESP wireframe was developed, discussed with partners and improved accordingly.
- Development of a new ESP design that was presented to partners.
- Development of new content templates.

2.2.1 User interviews and UX recommendations

User interviews are a valuable research method for improving website user experience and an important part of the product development process, as they provide insights into users' needs, behaviours and motivations. The user interview is a UX research method in which a researcher asks questions about a specific topic in a 1:1 conversation to learn how the user acts and thinks when using the service. A total of 8 interviews were conducted, including interviews with different backgrounds and employment covering the interests of EXCELLERAT target groups (HPC engineers for industrial and academic CFD applications, research scientists, Ph.D. students working in the research institution, application experts and researchers, GPU programmers, computer scientists in a private IT company, project managers in an ICT vendor company, assistant professors at universities, communication experts working in software vendors). After collecting all feedback through the interviews, the feedback was analysed and showed what content and features of the portal function worked very well and which parts or technical aspects need further improvement.

The main findings were:

- Users like the simplicity of the graphic design.
- Developers and engineers can easily find the services for their needs and understand detailed service descriptions.
- Event and training information is easy to find, and clearly presented.
- Entry point on the ESP landing page is quickly accessible for engineers or developers, meanwhile, academics, technology providers or students/wider public could not find the entry point for the services (do not know where to start searching).
- Most users would suggest the renaming of some sections, as they could not relate to the names such as “Sections” in the main menu or “Excellerat resource library”.
- Users are confused about where to request the service when looking at the service description. Most users missed the “Request service” button.
- Some service descriptions need improvement as some types of users (e.g. academics, researchers, HPC providers) are missing some information for their purposes.
- Most users suggested to include the description of the services in the main service dashboard.
- Some technical issues occurred while having interviews – e.g. some windows and service descriptions are overlapping when using different devices (responsive design improvement needed), some links do not work, tags do not work.

According to the results, the UX team prepared recommendations how to improve the portal to meet the user needs, improve the content, its accessibility as well as the technical functionalities. The following sections improvement recommendations were addressed:

- Landing page
- Service list page and detailed service page
- Partners page

- Events page
- Training page
- Navigation
- Breadcrumbs (site map)
- Dashboards
- General Portal recommendation
- Design recommendation, including responsive design

2.2.2 Graphic design

The new ESP graphic design was developed, implementing UX recommendations and feedbacks from EXCELLERAT partners. By balancing aesthetics with user-friendly features, an appealing design was developed that serves the needs of the target users.

The new ESP will be aligned with the EXCELLERAT Visual Identity and will keep a clear, simple interface. It will offer the entry point to the services on the top. The dashboards entry points were removed; thus, users could directly enter to service list, and search for services.

The “Training and events” and “Repositories” sections follows.

The main menu of the new Portal offers: “Services”, “Collaboration”, “Training and Events”, “Repositories” and “Login” choices, can be seen on top of the Service Portal entry page in Figure 3. Service contents will be re-written and adapted, providing main information for users in the first plan. Additionally, the content is inviting users to explore and request services more directly, as it is re-written in more call-to-action format, as shown in Figure 4. In Figure 5, an example of a code detailed page is shown, which can be accessed from the previous mentioned service page. The design is responsive, this means, the ESP could perfectly fit and work for different digital devices.

Users who would like to request services or access to training materials will need to create a user account, which will be verified automatically through two-step verification due to security reasons.

The portal will be further developed in the next months by our partner Arctur and will remain accessible at the same domain name.

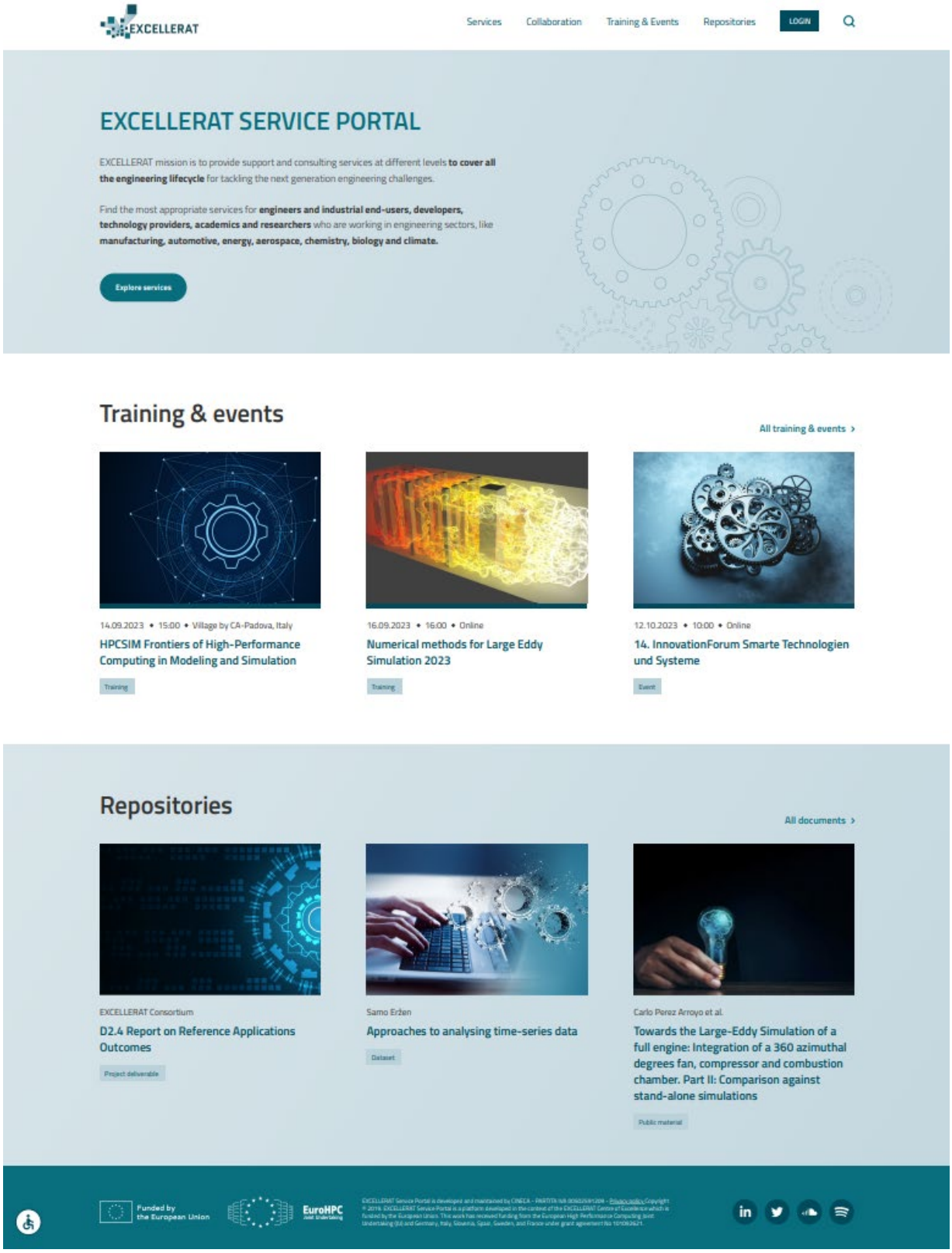

Figure 3: EXCELLERAT Portal design concept - Entry page

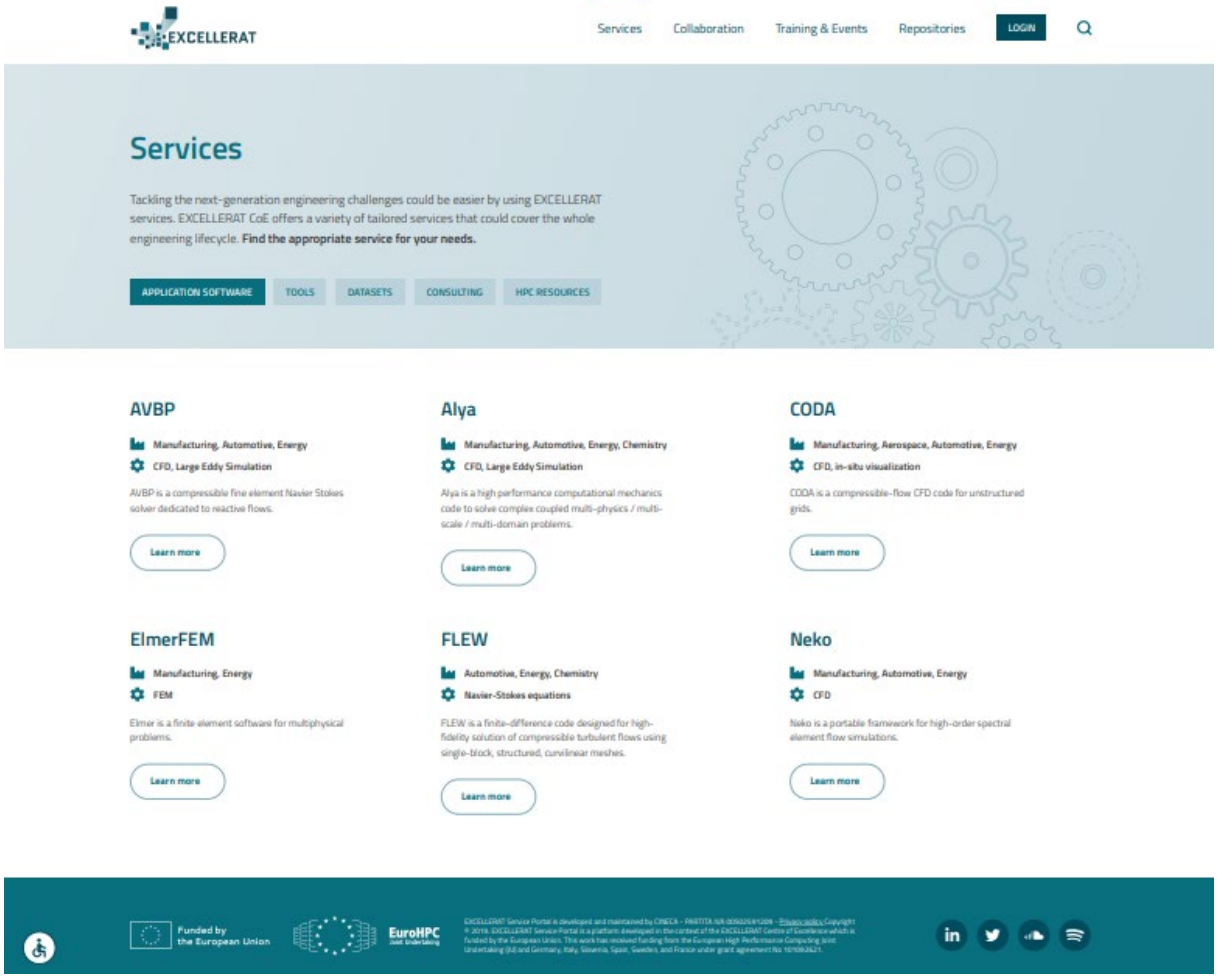

Figure 4: EXCELLERAT Portal design concept: Service Page

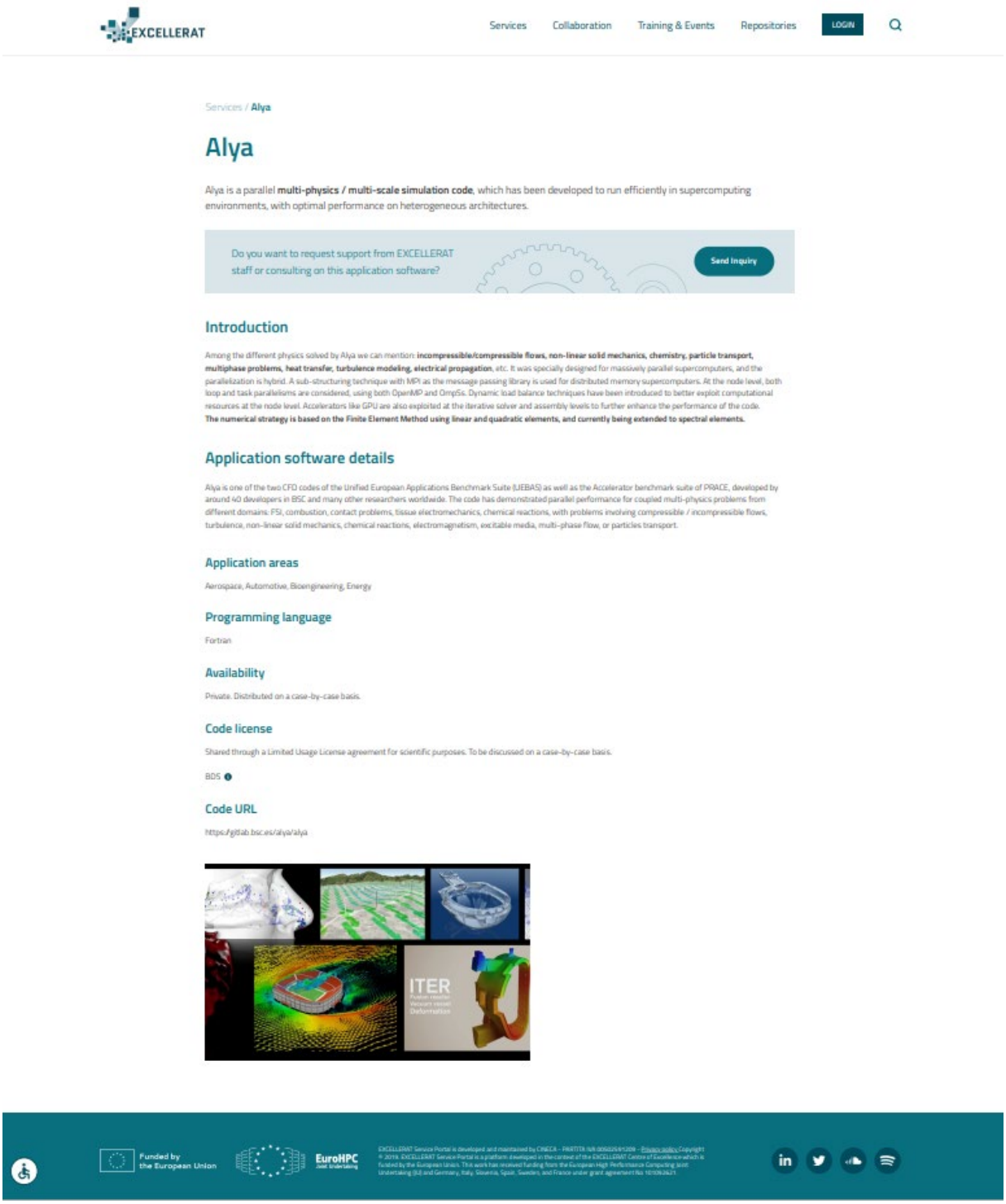

Figure 5: EXCELLERAT Portal design concept: Code Detailed Page

2.3 Future Outlook

The ESP development was planned for M1-M12, with its release in M12 (December 2023). However, the analysis part and content development took more time as planned. The reason is two-folded:

- The ESP is aligned with the project service list as defined in EXCELLERAT P1. It will be revised, improved and updated during the EXCELLERAT P2 phase with new services. The idea is to invite also external service providers (other CoEs, HPC and technology providers, ISVs, other research institutions), to offer their services on the ESP. The future service offering and onboarding of external providers have not been

defined during the time of the new ESP development, thus developing the ESP prototype took more time than planned. External providers and their services could be added later, when the strategy and guidelines will be defined

- The EXCELLERAT Consortium was informed that the new CI2SS Platform has been developed under the CASTIEL 2 auspices, and CoEs portals could become part of it, or at least, will exchange particular contents (potentially through the APIs) between the CI2SS and ESP. As there was no clear information provided during the ESP planning, and the connection with the CI2SS could seriously impact the ESP (re)-development in the later phases, the consortium decided to postpone further portal planning until all necessary information is received.

Due to the above-mentioned blockers, the ESP could be officially released some months later than planned (by February 2024).

3 Training and Education

This section has the following structure: in sub-section 3.1 we list all the EXCELLERAT P2 training events organised in Q2 and Q3 of 2023; in sub-section 3.2 we analyse the Key Performance Indicators (KPI) relative to the trainings; in the last sub-section we give an outlook on the future plans.

3.1 Training events

EXCELLERAT P2's training activities are designed to fill specific gaps in the offerings of our partner institutions. This means that we consider audience demand and the results of training evaluations when developing new activities. For example, we integrate interdisciplinary aspects specific to EXCELLERAT into established activities offered by consortium members. In addition, training on the flagship codes and associated tools will be provided either by EXCELLERAT experts or Interest Groups. EXCELLERAT P2 focuses on the field of engineering, but continues the outcomes of EXCELLERAT P1 as a focal point for the engineering community in Europe. Therefore, the training modules on data analysis for simulations developed by FhG in EXCELLERAT P1 have been adapted to the new developments. On a technical level, we see that not only High-Performance Computing (HPC), but also High-Performance Data Analytics and Artificial Intelligence (AI) courses are becoming more and more important in the engineering communities at application (software) and technology (hardware) level. Among other applications covered in this assignment, special attention is given to visualisation. Due to these project goals, we have streamlined our training program in 2023 in comparison to the training activities in 2020-2022, which has resulted in a slight decrease in the number of trainings. This optimisation allows us to provide more targeted and effective training experiences.

Since EXCELLERAT P2 is the continuation of the setup of EXCELLERAT P1, the respective training category stay unchanged and defined as it was introduced in EXCELLERAT P1:

- Parallel Programming [PAR]
- Computational Fluid Dynamics [CFD]
- Scientific Visualisation [VIS]
- Compute Cluster: Usage and administration [CLU]
- Performance Optimisation and Debugging [PRF]
- Data in HPC [DAT]
- Programming Languages for Scientific Computing [LNG]
- Scientific Conferences and Workshops [C+W]
- Training for special communities [COM]
- Others [OTH]

Table 1 provides a summary of the EXCELLERAT P2 training events that have taken place in Q2-Q3.

Quarter	Date	Training event	Training category	Type	Number of participants
Q2	April 17-21, 2023	Numerical methods for Large Eddy Simulation	CFD	Online	22
	June 5-7, 2023	From Machine Learning to Deep Learning: A concise introduction	DAT	Online	26
	June 12-14,	Data analytics for engineering data using machine learning	DAT	Online	18

	2023	2023-ML4SIM1			
Q3	October 9-10, 2023	Scientific Visualisation with COVISE and Vistle 2023-VIS1	VIS	On-site at USTUTT	14

Table 1: Conducted trainings for Task 5.2

In M1-12, the training effort below has been conducted. For each activity, these characteristics are specified: format, date, training category as above ([PAR] etc.), short description, resulting collaborations and material.

- "Numerical methods for Large Eddy Simulation" [CFD] (online from 2023-04-17 to 2023-04-21): This is a third edition of the 2021 CERFACS training on the EXCELLERAT flagship code AVBP to solve compressible Navier-Stokes equations for laminar and turbulent reactive flows, in 2D and 3D, on unstructured and hybrid meshes, with third-order Taylor-Galerkin schemes.
- "From Machine Learning to Deep Learning: A concise introduction" [DAT] (online from 2023-06-05 to 2023-06-07): This course addresses students, data scientists, and researchers who would like to have an introduction to machine and deep learning methods to solve challenging and future-oriented problems. The first part is an introduction to basic methods in Machine Learning (ML), including pre-processing and supervised learning using Apache Spark. In the second part, the course includes the elements of supervised Deep Learning (DL) on real data to classify annotated images of the waste in the wild. Given the deluge of information needed to power machine and deep learning methods, the course concluded with an introduction to data compression using the BigWhoop library (developed within EXCELLERAT P2) - an efficient data reduction tool, which can be applied to generic numerical datasets to minimise I/O bottlenecks and optimise data storage. The lectures are interleaved with many hands-on sessions using Jupyter notebooks and scripts on HLRS systems. In addition, a guest lecture from the Institute of Aerodynamics and Gas Dynamics (IAG), University of Stuttgart, showed how deep learning can be applied to problems in computational fluid dynamics.
- "Data analytics for engineering data using machine learning 2023-ML4SIM1" [DAT] (online from 2023-06-12 to 2023-06-14): After evaluating the participants' feedback of the previous course instances in order to optimise the learning outcome, the online Fraunhofer SCAI workshop will be offered one more time as a three-day course. Fraunhofer SCAI in cooperation with HLRS offered a third instance of the workshop addressing the preparation, analysis and interpretation of numerical simulation data by machine learning methods. Besides the introduction of the concepts such as clustering, dimensionality reduction, visualisation and prediction, this course provided hands-on tutorials using the libraries *numpy*, *scikit-learn* and *pytorch* as well as the Fraunhofer SCAI tool *SimExplore*. Since the second edition, the workshop has been extended to three days dedicated to prediction with deep learning, and to the interpretability of machine and deep learning methods. Material: The Jupyter notebooks used for the hands-on sessions can be downloaded from the Service Portal and executed locally or on a cluster. The main target group of these further instances are industrial end-users, e.g. belonging to the EXCELLERAT Interest Groups or to the EXCELLERAT partners' stakeholders.
- "Scientific Visualisation with COVISE and Vistle" [VIS] (on-site at USTUTT from 2023-10-09 to 2023-10-10): This will be the 2023 edition of the analogous visualisation course described in Section 4.2 of the deliverable D5.7 of the EXCELLERAT P1.

3.2 KPIs Analysis

Concerning the KPIs collection, we start from those defined for EXCELLERAT P1 in the deliverable D5.1 *"Initial Assessment of Training Needs and Services Building Plan"*.

Table 2 gives an overview of the KPIs for training events in the reporting period. Unfortunately, the KPI table is not complete because the KPIs from the last EXCELLERAT P2 training event are still missing. This event was on October 10th, and at the current time of this report, we still have not received all the feedback to our survey.

KPI number	Description	Definition	Target	Score at M40
5.2.1	Number (total) of participants in trainings of EXCELLERAT P2 (per year).	*N_{tota in yearl} = Sum_{1}^{n} N_{training,i}*	150/year	22 + 26 + 18 + 14 = 80
5.2.2	Balanced participation of males, females in EXCELLERAT P2 trainings. Gender ratio of the participant.	*N_female/N_total or R_female_male_quotient*	26% of female/non-binary	27%
5.2.3	ACSI score: Overall training satisfaction as average per year (via survey/feedback sheet).	N_{acsi}_training_per_year The scale is from 0 to 10.	7.5	8.5
5.2.4	The recommendation scale as average per year (via survey/feedback sheet).	N_{acsi}_recom_per_year The scale is YES or NO.	75%	79%

Table 2: KPIs for training events

All training KPIs were measured using an online survey. The evaluation was positive, but despite the advertising campaign carried out with the support of WP5, the number of course participants remained below the target value. Analysing the answers given by the participants will provide us with relevant and interesting observations.

KPI 5.2.1 ("Number of participants") remains below target. Although many efforts were made to successfully advertise the training, it can be a challenge to find suitable time slots for the training that consider the availability of a diverse group of participants. This resulted in some people not being able to attend due to scheduling conflicts. In addition, we may have reached saturation for similar courses. This in turn may lead to a decrease in demand and registrations for the training programs.

KPI 5.2.2 ("Balanced participation of men") The training program took an inclusive approach that actively encouraged and welcomed the participation of individuals of all genders. This approach conveyed that the program was open to and supportive of all, which likely contributed to balanced participation. Training content and topics were structured to appeal to a wide range

of participants, regardless of gender. Content that is seen as relevant and valuable to a diverse audience can attract balanced participation. This helps us to achieve the target set for this KPI.

KPI 5.2.3 ("Overall training satisfaction") Overall, the feedback is positive, highlighting various aspects of the courses that were well-received by the participants.

- The instructors were highly regarded.
- Participants appreciated the flexibility of the online format for half-day workshops.
- The offered courses have a good balance between hands-on and theoretical content. Participants learned many new things and liked the course format.
- The courses were described as great, friendly, and useful.
- Many participants found the courses very good and well-suited to its duration.
- The fast pace and solutions walkthrough were enjoyed.
- The lecture content was deemed sufficient and well-organised.
- The interactive elements, engaging teaching methods, and accessibility of materials were appreciated.
- The course worked very well for the participants.

Participants had positive feedback about the training event's content and lecturers, highlighting various aspects they liked:

- The presenter's qualifications and explanation skills were well-received.
- The scope and choice of topics were praised.
- Participants appreciated the opportunity to work on actual applications and improve model accuracy through experimentation. Therefore, participants found the content engaging and relevant to their professional development.
- The materials were adapted for those with varying levels of familiarity with machine learning.
- The structure of the training was well-liked, and the content was comprehensive.
- The interactive exercises and activities were enjoyable and contributed to active participation.
- The Jupyter notebooks and lectures were particularly well-regarded.

In general, participants expressed a strong appreciation for the presenter's extensive qualifications, the depth of topics covered, the quality of materials provided, the effectiveness of exercises and activities, the well-structured nature of the training event, and the various hands-on sessions that enhanced the learning experience. They found the content to be not only engaging but also highly comprehensive, delivering valuable insights and skills essential for their professional development and ongoing research efforts.

KPI 5.2.4 ("The recommendation scale") The main aim to join the EXCELLERAT P2 trainings:

- Acquiring the ability to perform combustion calculations.
- Learning to conduct ABVP calculations with two-phase fluids.
- Gaining proficiency in utilizing AVBP and its tools.
- Combining theoretical and practical knowledge of AVBP to enhance efficiency.
- Launching Large Eddy Simulation (LES) reactive simulations.
- Attaining an overview of AVBP capabilities, such as 1D flame computations for ARC.
- Mastering AVBP basics for use in a Ph.D. project on RQL combustors.
- Learning data input setup (Mise en Données).
- Becoming comfortable with CERFACS tools and comprehending simulation procedures.

- Developing expertise in AVBP configuration and numerical models.
- Fostering familiarity with AVBP, identifying common use cases, and gaining competence in setting up and running simple cases.
- Expanding knowledge of AVBP and its tools.
- Understanding the practical usage of AVBP (discovering AVBP for various applications), enabling independent test case analysis.
- Gaining hands-on experience with AVBP.
- Enhancing knowledge of the software to conduct advanced simulations, including combustion studies, boundary conditions, and modelling of chemical species like H_2 and OH^*.

3.3 Outlook to the future

Task 5.2 is planning to conduct a new ML4SIM2 instance. Fraunhofer SCAI needs to consider who will be a next speaker. Plan to organise this course in the Q2 of 2024 or later.

The partners working on OpenFoam + RaySect Mitsuba2 are not planning any training yet.

Alya simulation code team plan to come up with the training program in the first part of 2024.

Participants expressed a range of interests for future training topics, including:

- Repeating the same course for better understanding.
- Topics related to 3D modelling and 3D printing.
- Automation and robotics.
- Physics-informed neural networks.
- Object-oriented programming.
- Advanced and State-of-the-art machine learning models and deep learning techniques and its applications. Parallelisation, and infectious disease modelling.
- In-depth insight into machine learning and deep learning.
- Transformer ML (ChatGPT).
- Application of ML/DL methods in earth science, including surrogate models.
- Application-oriented topics, such as finding surrogate models for FEM simulation.

Analysis of this feedback has been discussed on the CASTIEL WP3 meetings (31.10.23 and 07.11.23). The next steps involve conducting a comprehensive analysis of the entire pool of EuroCC2 experts to identify the most suitable candidate(s) who can effectively address the gaps in the training topics aligned with the objectives of the EXCELLERAT P2 project. At present, this remains an open question as the selected expert is expected not only to possess expertise in the specified topic but also to design training exercises and hands-on sessions that align with the overarching objectives of the EXCELLERAT P2 project.

4 Resource Acquisition

As delineated in the Grant Agreement [2], task 5.3, *Resource acquisition*, has the objective of implementing for the internal provisioning of the HPC services and resources needed by the other WPs of EXCELLERAT P2.

More generally, task 5.3 provides a link between the CoE and the European HPC infrastructure, with a special focus on pre-exascale EuroHPC clusters.

The aims of the task include maintaining an updated list of available services, offering a single access point for CoE members to access specific services, providing support and documentation, and ensuring that requests coming from the Consortium are handled by the service delivery functions of the HPC centres.

While a wide variety of services are available in each HPC centre's service catalogue, and their inclusion in the list offered to CoE members constitutes a long-term objective of the task, the initial focus will be on the provision of two main services:

- Allocation of CPU time for developers, debugging activities and planned CoE experiments
- User support on HPC systems.

In the past phase of the project, computational resources were provided to the Consortium by PRACE, as 0.5% of the total resources available for each PRACE call were reserved for Centres of Excellence such as EXCELLERAT.

However, this is no longer the case and, at the time of writing, a scheme for special access to computational resources by the CoEs is still in the process of being defined by the EuroHPC JU.

Considering this situation, the activities of task 5.3 for the first year have been surveying the use case owners from work package 2 for their experience and expectations regarding resource allocation, and interfacing with CASTIEL 2 to perform an overview of the access modes to computational resources provided by the JU and of the of the requirement estimates for the CoE.

4.1 Access modes to JU systems

EXCELLERAT P2 is one of the 10 HPC Centres of Excellence (CoEs) funded through the HORIZON-EUROHPC-JU-2021-COE-01 call. These CoEs collectively manage about 60 HPC codes/pilots, and for each code/pilot they need access to several JU systems.

The task of defining a special access scheme to HPC resources for CoEs was assigned to the JU flagship project CASTIEL 2.

4.1.1 *Different access schemes*

Access to EuroHPC JU systems is currently granted based on individual project applications and purpose types in four different access schemes:

- Benchmark
- Development
- Extreme
- Regular

4.1.2 *Resource requirements estimation*

The Coordination and Support Action (CSA) CASTIEL 2 was tasked with collecting requirements from the CoEs about the estimated resources needed for installation, testing, benchmarking, and development of their codes/pilots on different EuroHPC systems.

The collection began in February 2023 (M2 for EXCELLERAT P2) and involved collecting details for all codes/pilots, including installability on known systems, access categories, and required resources. Specific hardware and tool chain requirements were also collected. Estimates of requests were asked for all four years of the CoEs' lifetime, although numbers and planned access for the coming years are only indicative.

The requests align with the limits for individual applications.

The total requested core-hours by all CoEs for Year (Y) 1 are thus approximately:

- 230 M core-hours for benchmark access
- 270 M core-hours for development access
- 260 M core-hours for extreme access
- 320 M core-hours for regular access

The total requested core-hours by all CoEs for all types of access per year are:

- 1000 M core-hours for Y1 (2023)
- 1500 M core-hours for Y2 (2024)
- 5000 M core-hours for Y3 (2025)
- 6000 M core-hours for Y4 (2026)

Although the CoEs' requests were generally in line with what the systems offer through standard access procedures, it became apparent that the CoEs' input is marked by a high degree of uncertainty, primarily because the CoEs' activities are still in their early stages, and they lack first-hand experience with the majority of the JU systems (some of which are not yet offered). Therefore, for the sake of a quick and easy start of providing CoEs the needed access to the JU systems, a differentiated approach was suggested by CASTIEL 2:

- A "flat-rate" or "base-rate" approach for benchmark & development-type access, giving each code a set amount of resources (on all systems for benchmarking and on the selected ones for development), in order to facilitate quick access to gather the required technical experience and enable benchmarking runs on various machines
- An individualised but accelerated approach for regular and extreme access.

4.1.3 *EXCELLERAT P2 requirement estimates*

The core hour numbers collected by CASTIEL 2 are estimates and should be considered subject to changes (especially for years 2024-2026).

The estimates for the codes of EXCELLERAT P2's Work Package 2 are reported in Table 3 to Table 6. All estimates were provided by CASTIEL 2 except for the FLEW use case (numbers in red in the tables), as the code owner provided task 5.3 with updated figures in June 2023 (M6).

	BENCHMARK			
CODE	**Year 1**	**Year 2**	**Year 3**	**Year 4**
m-AIA	1.500.000	1.500.000	2.500.000	2.500.000
AVBP	100.000	200.000	500.000	500.000
Neko	5.150.000	5.150.000	5.150.000	5.150.000
Alya	2.000	4.000	0	0
CODA	100.000	100.000	200.000	200.000
OpenFOAM	515.000	515.000	515.000	0
Mitsuba2	515.000	515.000	515.000	0
FLEW	515.000	1.030.000	1.030.000	1.030.000
TOTAL	**15.092.000**	**18.284.000**	**21.740.000**	**20.710.000**

Table 3: Resource requirements for EXCELLERAT P2 codes/use cases for BENCHMARK access

	DEVELOPMENT			
CODE	**Year 1**	**Year 2**	**Year 3**	**Year 4**
m-AIA	500.000	500.000	1.000.000	1.000.000
AVBP	500.000	500.000	500.000	500.000
Neko	10.300.000	10.300.000	10.300.000	10.300.000
Alya	0	20.000	40.000	40.000
CODA	25.000	50.000	75.000	100.000
OpenFOAM	1.030.000	1.030.000	1.030.000	1.030.000
Mitsuba2	1.030.000	1.030.000	1.030.000	1.030.000
FLEW	515.000	1.030.000	1.030.000	1.030.000
TOTAL	**19.565.000**	**19.610.000**	**20.155.000**	**17.090.000**

Table 4: Resource requirements for EXCELLERAT P2 codes/use cases for DEVELOPMENT access

	EXTREME			
CODE	**Year 1**	**Year 2**	**Year 3**	**Year 4**
m-AIA	3.000.000	3.000.000	5.000.000	5.000.000
AVBP	0	0	50.000.000	50.000.000
Neko	4.575.000	9.150.000	22.875.000	22.875.000
Alya	0	500.000	2.000.000	8.000.000
CODA	0	0	1.000.000	1.000.000
OpenFOAM	0	0	0	20.600.000
Mitsuba2	0	0	0	15.450.000
FLEW	5.150.000	20.600.000	20.600.000	20.600.000
TOTAL	**12.725.000**	**22.950.000**	**183.875.000**	**225.925.000**

Table 5: Resource requirements for EXCELLERAT P2 codes/use cases for EXTREME access

	REGULAR			
CODE	**Year 1**	**Year 2**	**Year 3**	**Year 4**
m-AIA	1.500.000	1.500.000	3.000.000	3.000.000
AVBP	10.000.000	20.000.000	20.000.000	20.000.000
Neko	2.287.500	4.575.000	11.437.500	11.437.500
Alya	2.000.000	100.000	500.000	500.000
CODA	0	0	0	0
OpenFOAM	0	0	10.300.000	10.300.000
Mitsuba2	0	0	10.300.000	10.300.000
FLEW	2.060.000	8.240.000	8.240.000	8.240.000
TOTAL	**95.787.500**	**126.175.000**	**175.537.500**	**175.537.500**

Table 6: Resource requirements for EXCELLERAT P2 codes/use cases for REGULAR access

CASTIEL 2 recommended to update the tables regularly, ideally at the end of every calendar year.

4.2 Provisioning requests and allocations

In June 2023 (M6) a survey was conducted by task 5.3 to gather information from the EXCELLERAT P2 code owners on their experience and expectations regarding the assignment of computational resources.

50% of the code owners answered the survey, a summary of the results is provided in Table 7.

Question	Answer
Did you apply to JU calls?	One applied outside EXCELLERAT P2, all others answered no, as they are waiting for the EuroHPC JU to define a special access scheme for CoEs.
Did you get resources other than from JU?	None applied for resources other than from the EuroHPC JU however, one cited using internal resources.
Do you have updates on your estimations with respect to the data provided to CASTIEL 2?	All respondents confirmed the validity of the estimates provided to CASTIEL 2, except for the owner of the FLEW code, who provided updated estimates, as reported Table 6.
Any comment with respect on what you expect from Task 5.3?	Other than coordinating computational resource allocation, some code owners requested additional information on how this can be achieved.
do you expect to apply to JU calls or to other HPC provisioning calls to perform your tasks?	Respondents indicated an interest in applying to other HPC provisioning calls adding, however, that they would prefer if resources could be provided through the CoE.

Table 7: Results of the June 2023 Task 5.3 survey

To summarise, most of them are waiting for the special access scheme for CoEs to be defined by the JU before applying for resources, as they would prefer to obtain access to computational resources through EXCELLERAT P2. Additionally, they asked for more information to be provided regarding the assignment process and the status of the special access scheme definition. This can be provided by task 5.3.

A second survey was performed in October 2023 (M10) by CASTIEL 2, the results for the EXCELLERAT P2 codes are summarised in Table 8.

Question	Answer
Which access calls have you used? (Benchmarking, Development, Regular, Extreme)	Benchmarking: 5 codes, Development: 1 code, Regular: 2 codes.
How many different codes were already executed successfully on at least one EuroHPC system?	8 codes.
Are the resources requested and assigned are sufficient to reach the objectives of your CoE? **Likely the resources will be sufficient for the first year. Can you already do a projection for the following years?**	Mostly all code owners state that resources are sufficient for the first year (2023), where the code is tested and benchmarked. But more resources will be needed from 2024 till the end of the project. BSC (Alya) estimates for next years: 2024 3M Core Hours, 2025 5MCore Hours, 2026 9M Core Hours. CINECA (Flew) estimates that about 1M GPU hours/year will be sufficient. 3 out of 7 code owners could not make any predictions.
Please report briefly about the experiences made on the EuroHPC systems? **How was the application process? Did you face any difficulties getting your codes to run? Did you get (technical) support by EuroHPC hosting sites if needed?**	The experience is overall positive. Application is smooth but bit too long to be granted access (over a month). Some technical support from Hosting Sites was given. One code owner reported different access procedures and conditions to each system, so it would be great to have a unique profile for EuroHPC users.
Can you please provide your feedback regarding the need of having a common GitLab and **give some preliminary information about what you would push to such repository? E.g. share** **the actual code, deployable software artefacts, binaries, deployment recipes, ...**	All have GitLab or Github repositories, one code owner has already GitLab runners to run the CICD pipelines. If required by CASTIEL 2 we are available to share the source code and deployment recipes, as docker/singularity images of the protected software (2 or 3 applications) and opensource packages (all).
Can you start deploying codes on a EuroHPC system in the next weeks using GitLab Runner?	Four answered yes, possibly testing the software stack beforehand; two answered no.

What will be your first code to share with the common GitLab server? Can you provide a timeline? (describe some technical limitations that you might face)	The non-opensource code cannot be uploaded as it is to the GitLab server without some information on the access policy. The opensource ones can be upload anytime. One code owner still needs to complete the development of the code (M18-M24), then will be ready to share code.
Do you have further feedback for us?	The GitLaB/CI requirement in this document seems to imply its coming from us whereas it was not on the original proposal. We can adapt to this situation, but a clarification seems in order. Also looking at the different EuroHPC hosting sites, support for GitLab CI and/or containers seems very heterogeneous. A panorama of support per system would be appreciated. It would be good to have the contact details to the technical support of the common GitLab server or the EuroHPC system.

Table 8: Results of the October 2023 CASTIEL 2 survey

To summarise, all eight codes have successfully been executed on at least one EuroHPC system, with most stating that the resources are sufficient for the first year (2023) but more are needed from 2024 until the project's end. The experience on EuroHPC systems is overall positive, with some complaints about long access times.

Interest in a shared GitLab or Github repository is mild, as all code owners already have repositories to share their developments.

On the other hand, code owners would be interested in having a unique application procedure for all EuroHPC systems.

5 Further Applications

This section is devoted to illustrating the current state of advancement of Task 5.4 "*Further Applications*".

Task 5.4 is responsible to ensure that new users or members of EXCELLERAT are going through the onboarding process and are closely integrated with EXCELLERAT's established procedures in terms of e.g. requirements assessment, application development or task integration.

After a successful onboarding, Task 2.4 will be responsible for progress monitoring and result generation for the use cases selected, following the methodology used in WP2.

The first use case monitored by this task is the realisation of the digital twin of the first wall of the ITER tokamak, in order to optimise this component of the tokamak. ITER (International Thermonuclear Experimental Reactor) is an international project with the scope of creating the first nuclear fusion reactor, where the tokamak is the torus-shaped device used to confine the plasma through strong magnetic fields.

Moreover, Task 5.4, together with Task 7.2, is responsible of the transfer of technical new competences relative to codes that are currently not part of EXCELLERAT´s competence offer towards the technical WPs.

A particular focus will be devoted to interactive on-site visualisation, namely providing installable downloads for Windows and documentation for remote visualisation client software on user machines.

Finally, Task 5.4 will monitor the development of large use cases, via frequent communication with the use case owners, in order to promptly react to new challenges.

This section has the following structure: in section 5.1, we will firstly outline the portal onboarding workflow; then we will continue in section 5.2 with the onboarding requests currently under consideration; in the last part, section 5.3, we will focus on the advancement in engineering the tokamak digital twin (see also deliverable D2.1 for a detailed description of this use case and section 8.5 for the summary of updates up to M12, detailed in deliverable D2.16).

5.1 EXCELLERAT portal onboarding workflow

There are several ways foreseen in EXCELLERAT to attract new applications and, thus, potential new end-users/customers:

- Via the interest groups
- Via the EXCELLERAT service portal.
- Via the EXCELLERAT awareness creation channels
- Via presentations by EXCELLERAT members through conferences and workshops.

During the previous project phase, the structural requirements for the service portal to attract external codes have been analysed, presented in EXCELLERAT P1 deliverables D5.1, D5.3, D5.5 and D5.7. The onboarding procedure has been implemented in the service portal. The revision and update of the service portal under elaboration by Task 5.1 requires some modifications in the workflow, that will be discussed here. The old workflow remains in use until the new portal enters the production phase. The following description refers to the updated service portal.

After successful registration to the portal, the applicant creates an onboarding request by compiling and submitting a provided form. This form, under implementation, contains all fields necessary to get a clear view of the kind of request: general description of the application, technical and scientific domain, methodology so far applied, envisaged or ongoing applications, current scalability performance, already detected bottlenecks, whether the application is fully or partially under NDA, etc. The form should be thorough enough to avoid too high a number of further inquiries. For this reason, it will be elaborated by WP5 together with the technical WPs and, if necessary, the Project Management Team (PMT).

After submission, the second step is carried out by an evaluation team composed by a team composed of three experts, representing and selected by the PMT, WP5 and the three technical work packages: 2 *"Use-Case Execution"*, 3 *"Exa-HPC Methodologies and Technology"*, 4 *"Workflow Development"*. General evaluation criteria include a feasibility checklist to pre-screen the application, and at least one partner having effort and interest to work on the submitted code. The evaluation might involve the request of additional information via tele-conferences or emails and should be concluded within a specified timeframe.

In case of positive evaluation, both, the partner selected for collaboration and the applicant, will receive a template for their "onboarded application software" to provide the information to be

displayed on the portal. The applicant will also decide which results and advances they would like to post on the EXCELLERAT portal during the joint work.

Within a specified timeframe, the designated EXCELLERAT partner will produce a workplan with a time-schedule and submit it to the applicant.

In case of negative evaluation, the applicant will receive a message, containing an explanation of the rejection.

Metrics for the evaluation are the impact factor on the community, the availability of the code, e.g. open-source, the quality of the technical preparation of the request, the availability of the later results, e.g. in a scientific data base, the aimed core count of the production run, and the expected scalability.

Each request is handled as a single project internally. To simplify the communication process, each project is managed by the group of experts who are currently working on the specific challenge. The targeted lead time for each project should not exceed 3 months.

5.2 Onboarding requests under consideration

NCC Austria forwarded EXCELLERAT a request from a local SME ISV DCS Computing GmbH.

DCS produces a software, Aspherix [5], for modelling complex fluid-particle processes using the Discrete Elements Method (DEM) and coupled CFD-DEM. They wanted to explore the opportunities offered by porting the solver to GPU for increasing the solver performance, and they already identified Kokkos [6], a C++ Performance Portability EcoSystem library, as the most promising tool since it was already successfully adopted in LAMMPS, from which Aspherix is derived. The SME however lacked the internal expertise in GPU porting and in using Kokkos in particular.

The request is under evaluation.

5.3 Tokamak digital twin

The first further application-case of the project consists of engineering the digital twin of the first wall of a tokamak fusion reactor, namely that part of the fusion reactor assigned to the confinement of the plasma. The scope of creating the tokamak digital twin is to better design and optimise this crucial component of the fusion reactor. Along this, the digital twin allows to reach a deeper understanding of the physical processes around the inner wall during the fusion reactions, possible leading to real-time control of fusion reaction.

In more detail, one of the scopes is to constantly monitor the temperature distribution of the inner wall, thanks to infra-red cameras, to detect in real-time overheating parts allowing to react before any damage occurs.

To obtain this optimisation, the dependency of the tokamak performance with respect to the geometry and the temperature of the system is modelled with Finite Element Methods, i.e., via the Elmer FEM code and with Finite Volume Methods, i.e., via OpenFOAM. The results will be validated using experimental data that are available from ITER first plasma experiments (using a temporary limiter) and synthetic diagnostic that combines infra-red and visible light camera images.

The optical performance of visible light and infra-red cameras is simulated, based on Monte Carlo methods using forward ray-tracing algorithms to predict the optical flow. Optical parameters such as surface reflectivity are modelled with Cook-Torrance models, which are assessed with ray-tracing codes.

The goal of the simulations is to accurately predict stray light, hot spots and uniformity. Since cameras do see not only surface temperature, but reflected light from other surfaces as well, coupled thermal-optics simulations under high reflectance are used to correctly describe the visible light: when reflections are subtracted, correct surface temperatures are determined. Therefore, only complete simulations (namely, digital twins) can give correct results to be seen by cameras.

5.3.1 Workflow and challenges

The assessment of a synthetic image of this kind requires three numerical simulations to be executed in an ordered sequence, in the sense that the output of one simulation is the input of the following one. In particular, the simulations to be performed are, in time-sequence order:

- Field line tracing
- Thermal model
- Optical simulation

The last step of this simulations chain gives as output an image, called synthetic measurement. An example of the latter is given in Figure 6.

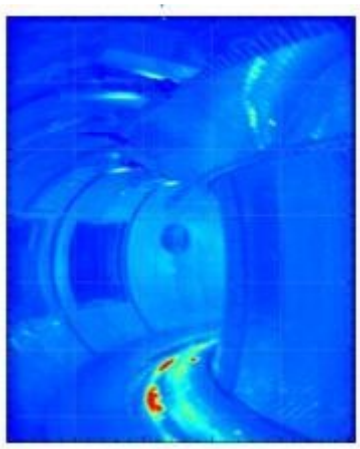

Figure 6: Synthetic camera image of WEST tokamak during operation

The main challenges of this simulations work concern the large size of the input/output data, i.e. for optical simulations a complete temperature distribution is needed, and the coordination of the different computational resources.

The described modelling work has been partially done at the University of Ljubljana (UL). Concerning what is still missing, mostly due to the need of porting the simulations to HPC systems. Access to Vega, namely to a peta-scale system, has been granted and access to LUMI, MareNostrum and Karolina is currently underway.

In the following we give a more technical description of the workflow, we include the current progress and the future steps of each simulation process.

5.3.2 Progress

We describe here the current advancement of the simulation processes, namely field line tracing, thermal modelling and optical simulation.

- Field line tracing:
  - Magnetic equilibria will be supplied by UL partners (ITER, CEA)
  - Field line tracing is assessed taking into the account the magnetic equilibria and 2D geometry.

  Advancement and outlook. The code L2G [4]] developed at UL and ITER has been optimised, the code improvement regards: octree space partitioning and bounding box partitioning of large meshes to decrease time of line triangle intersection checks. Moreover, the parallelisation of field line tracing is obtained by splitting the trace into multiple smaller traces for each field line. This parallelisation works on CPUs, the next step is to port it to GPUs.

- Thermal modelling:
  - Heat flux distribution on the first wall is provided and mapped on the simplified 3D geometry of the tokamak first wall.
  - Thermal model assesses the temperature distribution on the first wall.

  Advancement and outlook. A small scale was prepared based on ITER temporary limiter, in particular, one block of temporary limiter was the object of the study, which forms the basis for a large-scale scenario. In more detail, the temporary limiter block was studied with a 3D mesh of about 300k tetrahedrons and 230k triangles on the plasma facing component. Then the heat flux is mapped to the 3D model and the heat equation is solved using Nearest Neighbour Interpolation. The outcome is the temperature distribution on the surface, which will be the input for the optical simulation, as described in what follows.

- Optical simulation:
  - Temperature is given as input to the optical camera simulation.
  - Based on camera parameters and defined reflection and radiation on the wall (a function of the temperature) an optical simulation is performed, which returns synthetic camera image.

  Advancement and outlook. Given the temperatures for one block of temporary limiter, evaluated through the thermal modelling previously described, signals on IR camera were then calculated for camera resolution 640×512, field of view $21.7° \times 17.5°$ and pixel size of $15\mu m$ (see Fig. 5). The case consists of 48 different slices with $0.04s$ time step. At this stage, a simple ray-tracing simulation was performed with Raysect (currently running on multiple cores).

In Figure 7, we show the result of each simulation process just described. In the first square of the figure the field line tracing part is shown, namely one block of temporary limiter with one field line trace. In the second square we show the corresponding heat fluxes and temperatures evaluated through thermal modelling. The last square presents a result from the optical simulation, a pixelated image (as seen by camera) is shown, compared to initial temperature distribution from thermal model. The last plot shows the reconstructed temperature compared with the black cross-section line.

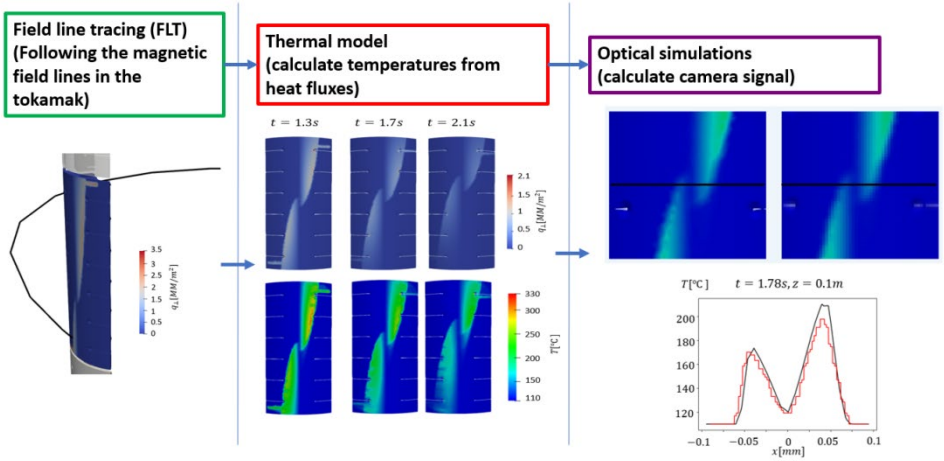

Figure 7: Small scale simulation setup

5.3.3 Work plan

Regarding the next steps, we attach the Gantt Chart in Figure 8 to show the progress plan expected for the tokamak digital twin: the goal for year 2 is to increase scalability and move to more complex cases for ITER operation considering components more advanced than temporary limiter. Moreover, the ITER first wall consists of about 440 panels which are actively cooled, whereas the temporary limiter block is not. As a consequence, the boundary conditions of the case will be modified by introducing this additional contribution to the heat transfer coefficient.

We also wrap up here the success criteria for this use case which are the following:

- Development of a workflow which outputs synthetic image without user interaction.
- Efficient usage of HPC hardware during the workflow execution (in terms of computational resources and data storage).
- Identification of hot spots on the first wall based on large scale simulation.
- Successful analysis of synthetic images to predict thermal loading on the first wall for a given magnetic equilibrium.

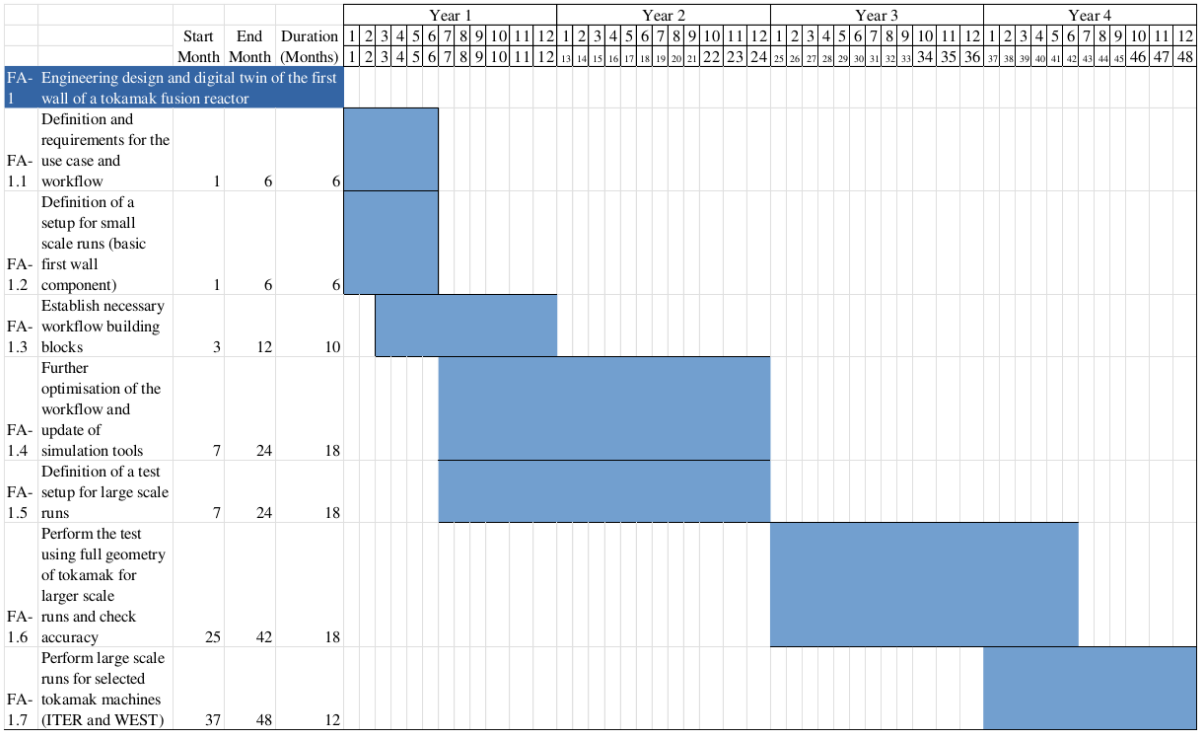

Figure 8: Gantt Chart for the tokamak digital twin

6 Conclusion

In this document we addressed the advancement state and the future outlooks of the four tasks of work package 5. We summarise here the main contents.

Task 5.1 *Service Provisioning*: the new EXCELLERAT Service Portal graphic design has been developed according to the result of the satisfaction survey of the users. The new portal will be developed in the next months by CoE partner ARCTUR.

Task 5.2 *Training and Education*: four main training events have taken place during the first 10 months of the project, it is possible to find in section 3.2 the related KPI analysis. Overall, the training event contents and lectures received positive feedbacks from the participants. A new machine learning course is currently being organised and it will probably take place at the beginning of 2024.

Task 5.3 *Resource Acquisition*: as the EuroHPC JU has not yet defined a special access scheme to computational resources for Centres of Excellence, the activity of task 5.3 for the first year consisted mainly collecting information in collaboration with CASTIEL 2. The computational requirements of the various EXCELLERAT P2 use cases were estimated, and input from the code owners concerning the service offerings collected.

Task 5.4 *Further Applications*: The application form for the onboarding of new applications through the service portal is currently being developed. In the meantime, task 5.4 has been collaborating with the technical WPs in following the first onboarded use case, the digital twin of the first wall of a tokamak fusion reactor, which is currently proceeding on schedule. Additionally, an onboarding request from DCS Computing GmbH forwarded by the Austrian NCC is being evaluated.

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