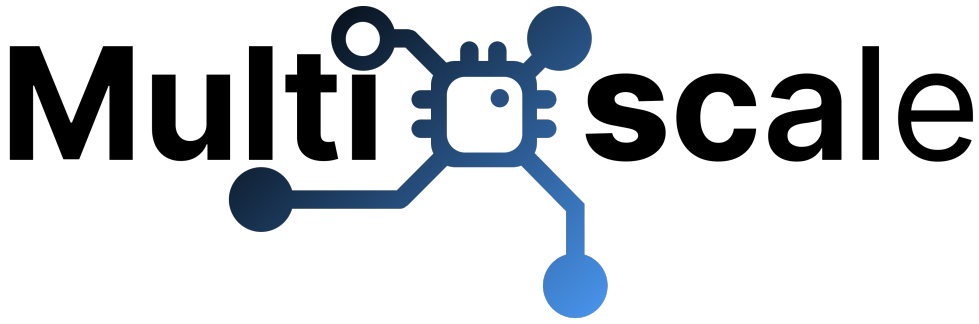

Project collaboration plan

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EuroHPC Centre of Excellence for
Multiscale Modelling

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Executive Summary

This deliverable outlines the comprehensive plan of how MultiXscale will establish and nurture collaborative relationships both within the project team and with the wider The European High-Performance Computing (EuroHPC) ecosystem, associated partners, and supporters. The document defines common objectives and delineates various collaboration activities aimed at achieving shared goals and maximizing the project's impact on the high-performance computing landscape.

- **Internal Collaborations** (Section 2) outlines collaborations in the MultiXscale project achieved through its various work packages. It is divided into Scientific and Technical collaboration, Cross-cutting collaboration and collaboration with Associated Partners.
  - In the MultiXscale's **Scientific collaboration**, the key objectives revolve around enhancing the capabilities of community codes and models for pre-exascale simulations, optimization of existing codes and the development of advanced software interfaces to enable seamless communication between different length scales and to create state-of-the-art pre-exascale workflows capable of conducting showcase simulations efficiently. **Collaboration activities in the scientific domain** are facilitated by the **participation of scientific partners in the CECAM network**, which allows for the cross-pollination of ideas and expertise. **Regular Scientific Virtual Team Meetings** (including WP2, WP3, WP4) are held to promote cohesion among project team members and serve as platforms to **discuss project progress, share insights, and collaboratively address challenges**.
    The primary focus in MultiXscale is to develop **applications that can efficiently run on petascale High Performance Computing (HPC) environments and prepare them for the exascale computing era**. As an example, the Extensible Simulation Package for Research on Soft Matter (ESPResSo) software serves as a case study in this endeavor. Partners are engaging in discussions to explore new approaches to parallel I/O and enhance the coupling of ESPResSo with waLBerla to create a reusable library for broader project use. This collaborative effort extends beyond ESPResSo and encompasses various applications. For instance, Kokkos is being leveraged in the development of an electrostatic solver that will be used by ESPResSo, within LAMMPS and (potentially) for a battery application at the University of Sorbonne. This aggregation of expertise in specific tools and methods facilitates extensive collaboration among MultiXscale partners.
    Furthermore, the University of Stuttgart, in collaboration with other MultiXscale partners, is actively working on identifying technical solutions to optimize ESPResSo's performance on pre-exascale systems. This optimization is especially relevant for applications like battery development, one of the experimental showcases within project WP4 at the University of Sorbonne. Additionally, MultiXscale involves the creation of high-performance and portable electrostatic solvers using Kokkos in collaboration with the Jülich Supercomputing Centre. Once completed, these solvers will be integrated into ESPResSo to enhance scalability in systems containing charged particles.
  - Within the **Technical collaboration** in the MultiXscale, the primary objectives are centered on **establishing the necessary infrastructure and services to support the European Environment for Scientific Software Installations (EESSI),** a pivotal component of the project. These objectives encompass the implementation of technical services required for EESSI delivery, expansion of EESSI's service offerings to incorporate CI capabilities for broader community benefit, development of tools to facilitate EESSI's rapid expansion through user contributions, and the facilitation of EESSI adoption by HPC sites, with a specific focus on EuroHPC sites. EESSI serves as the central hub for various technical activities within the MultiXscale project. These collaborative activities entail fostering cohesion and seamless communication among project team members through regular Technical Virtual Team Meetings, encompassing various Work Packages (WPs) such as WP1, WP5, WP6, and WP7. A number of partners collaborate to optimise the performance of the delivery mechanism used within EESSI, the CernVM File System. Activities in soft infrastructure are supporting software deployment within the EESSI environment which aligns with the interests of all partners, who aim to have their supported software environments integrated into EESSI.
    Active collaboration of partners is required in activities of architecture and application support, acknowledging that specific sites may have unique interests in particular architectures or applications they wish to incorporate into EESSI. Incorporating a software package into EESSI entails, to a reasonable extent, ensuring that it is capable of building and passing tests on all the supported architectures. Consequently, individuals interested in specific applications must also address hardware-related issues, while those handling hardware concerns must engage with the realm of applications. Open lines of communication among the entire technical partner group is essential for effective collaboration.
    Furthermore, technical support for users is an integral part of MultiXscale, with partners taking turns to provide support. Handover meetings and regular group meetings serve as platforms to address open tickets and provide opportunities for collaboration, ultimately leading to improvements in EESSI services.

  - **Cross-cutting collaboration** in MultiXscale is driven by common objectives that span both advancing HPC technologies and facilitating knowledge dissemination. These objectives include the collaborative development and refinement of HPC technologies, coordination and strengthening of the Center of Excellence (CoE) initiative at a pan-European level, maximizing impact on the European HPC user base, sharing research findings and methodologies with the wider scientific community, strengthening the EuroHPC landscape, and supporting collaboration, knowledge sharing, and best practices dissemination. Collaboration activities in this domain involve the integration of scientific application and workflows into EESSI, help with the development of tests for *marquee* applications to ensure correctness, scalability, and performance by scientific partners as well as contributions from them to user support services. Additionally, Continuous Integration (CI) services have been established to support application developers by EESSI.
    Dissemination efforts aim to promote MultiXscale through various means, for example a shared "elevator pitch" presentation to give all project partners an engaging, quick but comprehensive set of presentation materials that they can use to briefly present MultiXscale at any relevant activity they participate in. From a dissemination perspective there are many shared activities that will be undertaken including virtual meetings, collaborative publications, workshops, tutorials and other community engagement.
  - **Collaboration with associated partners** are primarily driven by specific goals related to the particular pilots of the project, as outlined in the project's Description of the action (DoA). As the project progresses, the scope of "Associated Partners" is intended to expand beyond its strict legal definition within the DoA. The project aims to engage in targeted collaborations with specific entities, recognizing their contributions to MultiXscale's objectives. MultiXscale recognizes the value of engaging with associated partners and supporters within academic institutions and research organizations to foster knowledge exchange and access complementary expertise. Showcases for this type of collaboration are in the DoA, such as engagements with the Université Paul Sabatier Toulouse III, specializing in multiscale modeling of supercapacitors, and the Max-Planck Institute, known for algorithmic expertise in lattice-Boltzmann and molecular dynamics simulations.
    Potential additional activities include direct collaboration with external community application developers to allow them to leverage the development infrastructure that EESSI provides, collaboration with HPC providers to offer EESSI as a software stack, and collaboration with community scientists to enable the deployment of their workflows within EESSI to facilitate broader adoption.

- **Collaboration with CoEs, Associated Partners and Supporters in the EuroHPC Ecosystem** (Section 3) outlines the collaboration within MultiXscale encompasses a broad spectrum of objectives and activities involving various partners and entities. MultiXscale's foundation lies in collaborative efforts within the HPC ecosystem. It brings together technical experts from Tier 0, 1, and 2 HPC centers through the EESSI and combines this expertise with the scientific proficiency of the Centre Européen de Calcul Atomique et Moléculaire (CECAM) network. The project has robust connections and collaborations with legacy projects such as PRACE, CASTIEL, and Fenix-RI, inheriting the legacy of the E-CAM Centre of Excellence. It also collaborates with partners engaged in EuroHPC infrastructure projects and National HPC Competence Centers.

  - One significant initiative is the **Ambassador Program**, aimed at nurturing the next generation of HPC experts and raising standards of competence in HPC provision. MultiXscale continues fruitful partnerships initiated by E-CAM, particularly in application development and training endeavors. The Ambassador Program for CECAM nodes and National Competence Centre for High Performance Computings (NCCs) is in progress and is committed to reaching and supporting user communities across EuroHPC countries and beyond, ensuring widespread access to its advancements and expertise. Ambassador program offers users guidance and direction on how to prepare for exascale computing (WP6) and equips them with the necessary tools for this purpose (WPs 1-5). Our software delivery approach is designed to ensure that researchers in European Union countries that are currently in the process of developing and advancing their HPC infrastructure can leverage the advancements made by the Center of Excellence, regardless of the current state of their national HPC facilities.

  - **Collaboration with CASTIEL2** MultiXscale collaborates actively with CASTIEL 2 which mission is to harmonize and reinforce the efforts of NCC and CoE initiatives across Europe. Its primary aim is to promote collaboration between NCCs and CoEs, enhancing their impact on European HPC and its user community. CASTIEL 2 seeks to consolidate the collective influence of CoEs and NCCs by nurturing networks, facilitating interaction, and addressing disparities in HPC expertise among countries. It also intends to expand the EuroCC Access portal into a comprehensive resource for EuroHPC expertise, software, training, events, and services.
    Within MultiXscale, champions have been designated for each WP in CASTIEL 2 to facilitate collaboration:
    "CASTIEL 2 WP2 - Networking & Competence": Matej Praprotnik (NIC) & Ignacio Pagonabarraga (UB);
    "CASTIEL 2 WP3 - Training": Alan O'Cais (UB);
    "CASTIEL 2 WP4 - Industry": Antonio Scirappa and Carlo Cavazzoni (both LEONARDO) and

"CASTIEL 2WP5 - Communication": Elisabeth Ortega and Susana Hernandez (both HPCNow!).
CoEs not only collaborate with CASTIEL 2 but also among themselves, with CASTIEL 2 fostering this collaboration. Various information is shared between CASTIEL2 and the CoEs, including CAB meeting materials, event invitations, competence and service maps, training activities, HPC in Europe portal, deliverables, access to CoE DoA, industry interaction, communication, minutes and presentations.
CoEs actively contribute to the knowledge pool and information to the common portal Cloud Cyber Intelligent Security Software (C2ISS); establish collaborations; participate in meetings to plan, implement and monitor collaborations and to synchronize research and development activities; contribute supported codes in the common continuous integration and application deployment platform with automated testing on all EuroHPC JU systems; establish common best practices for IP management and development; engage in modularization efforts, and contribute to bench-marking exercises; disseminate results and participate on joint events.
The goal is to facilitate knowledge exchange and joint efforts in addressing cross-cutting issues, ultimately strengthening the collaborative ties between CoEs and NCCs.

– **Collaboration with Industry** While industrial collaboration is not central to MultiXscale, existing activities hold substantial potential for growth. The objectives of collaboration with industry include advertising and facilitating the adoption of MultiXscale's solutions among industrial communities, assisting industrial users in adapting to new architectures, and creating tools and workflows to facilitate the adoption of EESSI in cloud environments. Two industrial partners, Leonardo and HPCnow!, participate in MultiXscale, contributing to both scientific and technical aspects.
Additionally, MultiXscale receives substantial in-kind support from Azure and AWS, as they recognize the game-changing potential of EESSI in supporting applications within cloud environments. EESSI ensures a consistent user experience across various architectures and offers a stable platform for providing additional application solutions.

These collaborations reflect MultiXscale's commitment to advancing HPC technologies, fostering knowledge dissemination, strengthening EuroHPC, and engaging with various partners to achieve its ambitious objectives.

1 Introduction

Most scientific groups that develop, implement, validate, and apply multiscale modelling approaches generally lack the human resources for the development of easy-to-use and versatile code for various platforms as well as the user base that is required for thorough validation. This reflects both the novelty of the field and the diversity of the approaches that are currently proposed and tested, and results in a situation where newcomers with an interest in particular techniques have to rely on the information found in scientific publications that generally provide neither sufficient insight to judge their applicability for other systems nor contain all the information needed to get started.

When addressing multiple scales there are significant methodological challenges, including algorithm design for horizontal coupling of scales (where all scales are simulated at once) and mapping techniques for vertical coupling (distinct, but coupled, simulations at different scales, with each scale posing different simulation challenges). In vertical coupling, there are the additional impacts of the coarsening that is typically carried out when moving between scales which requires the scientific validation of the resulting model. The current lack of scalable computational tools and coupling frameworks for these approaches makes it obvious that there is a high need for their development in order to make HPC attractive both for academic and industrial users. These users are frequently dealing with real world complex systems, presenting complex levels of length- and time-scale coupling but with high societal impact, e.g. in chemical- or pharmacological-industry. biomedicine or materials design.

It is with these challenges in mind that MultiXscale frames it's approach to collaboration both internally and externally. MultiXscale wishes to make as easy as possible to adopt the approaches developed by the project, adapt them to the end user case and implement on the computational resources they have access to. All of this while keeping the technical burden for users during this process at an easily manageable level.

1.1 Scope of the deliverable

This deliverable outlines a wide range of collaborative activities, both internal and external, that are either being implemented or planned within the MultiXscale CoE. These activities are crucial to the success of the project, and also ensure that the impact of the MultiXscale project within the EuroHPC ecosystem extends far beyond the project partners.

It highlights efforts to enhance software scalability and architecture support, foster partnerships with developers and end-users in the community, and leverage the European Environment for Scientific Software Installations (EESSI) to ensure the feedback loop between software developers and software end users can be significantly tightened.

In particular, we highlight EESSI as a means for the project to collaborate far beyond project partners and provide a service that has significant impact both in the target scientific community and also the broader HPC community.

1.2 Target audience

The content of this document is intended for the partners within the MultiXscale project, the CoEs with whom we are collaborating, CASTIEL 2 and a wider audience of the HPC environment, particularly in the EuroHPC ecosystem.

2 Internal Collaborations

MultiXscale is made up of two equally important core aspects:

- a scientific component focused on the development of multiscale software with specific scientific goals, and which can run efficiently at scale on EuroHPC hardware; and
- a technical component which implements the technical infrastructure to facilitate application development and deployment (and the deployment of the scientific workflows of which they form a part) into the hands of the scientific community as quickly as possible for all architectures they have access to.

2.1 Scientific Collaboration

2.1.1 Collaboration objectives

The essential objectives of the scientific collaboration within MultiXscale is to:

- Prepare and optimize existing community codes and models that are pertinent to MultiXscale project for pre-exascale simulations.
- Develop sophisticated software interfaces that facilitate seamless communication between different length scales, both within and between community codes. These interfaces will enable computationally efficient multiscale simulations, whether executed concurrently or sequentially.
- Provide state-of-the-art pre-exascale workflows that are capable of performing showcase simulations.
- Employ cutting-edge multiscale and multiphysics computational methods, ensuring their efficient implementation on pre-exascale architectures.

2.1.2 Collaboration activities

Through their participation in the CECAM network, the scientific partners are very familiar with each others work and scientific focus. MultiXscale resources the cross-pollination between these colleagues, examples of which include:

- Fostering cohesion and seamless communication among project team members through regular Scientific (including WP2, WP3, WP4) Virtual Team Meetings. These are scheduled to discuss project progress, share insights, and address challenges collaboratively and through other tools described in "D8.1 - Project Management methods and tools".
- The focus is on the development of the applications to align with one of MultiXscale's goals, **to run efficiently in petascale HPC environments and be ready for exascale computing**. Using ESPResSo software as an example, discussion with partners has resulted in them considering new approaches to parallel I/O, and also to making an enhanced effort to ensure that their coupling to "widely applicable lattice Boltzmann from Erlangen (waLBerla)" can be made available as a library for re-use within the project (and beyond). There are many potential similar examples, another of which is the use of Kokkos within the development of the electrostatic solver, as well as within Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS), and potentially the battery application being developed at the University of Sorbonne. Aggregating expertise in a particular tool or method opens the door to more extensive collaboration among partners.
- The development of ESPResSo at University of Stuttgart is identifying concrete technical solutions to make ESPResSo perform well on pre-exascale systems in collaboration with other MultiXscale partners which are studying its use in applications such as battery development (one of the experimental showcases in the project WP4 for University of Sorbonne).
- As part of MultiXscale, high-performance and portable electrostatic solvers are being created using Kokkos in collaboration with another scientific partner, Jülich Supercomputing Centre. Once available, these solvers will be used in ESPResSo to improve scalability in systems containing charged particles.

2.2 Technical Collaboration

2.2.1 Collaboration objectives

The essential objectives of the technical collaboration within MultiXscale is to:

- Put in place the technical services required to deliver EESSI.
- Expand the services offered by EESSI to include CI capabilities that can be offered to the community.

- Put in place the tooling to allow EESSI to grow quickly with user contributions.
- Facilitate the adoption of EESSI by HPC sites, and EuroHPC sites in particular.

2.2.2 Collaboration activities

The technical partners are similarly familiar with each other through their collaboration in EESSI. EESSI itself acts as the aggregation point for the various technical activities of the project. Such activities include:

- Fostering cohesion and seamless communication among project team members through regular Technical (including WP1, WP5, WP6 and WP7) Virtual Team Meetings. These are scheduled to discuss project progress, share insights, and address challenges collaboratively and through other tools described in "D8.1 - Project Management methods and tools".
- **Hard infrastructure** to support the delivery of EESSI. A number of partners collaborate to optimise the performance of the delivery mechanism used within EESSI, the CernVM File System. Since EESSI is designed to be expanded and customised by particular sites, localising expertise is of high value. This ensures active interest in collaboration.
- **Soft infrastructure** to support the deployment of software within the EESSI environment. All partners have a vested interest in this as they support software environments themselves which they hope to have supported within EESSI. Automating as much as possible the inclusion of software within EESSI is a short term cost in terms of effort, but will yield long term gains in terms of the expansion capability of EESSI.
- **Architecture and application support** also requires active collaboration of partners. Particular sites may have specific interest in certain architectures as that is what they host themselves or may have specific applications that they wish include in EESSI. The addition of a software package to EESSI requires (within reason) that it builds and passes tests on all supported architectures. This means that someone interested in an application needs to deal with hardware issues, and someone dealing with hardware needs to deal with the space of applications. No single person can cover all these matters and it is necessary to have open lines of communication among the entire group of technical partners
- **Technical support for users** is also part of MultiXscale. Partners are on rotation for support, with handover meetings between rotations and regular group meetings to discuss open tickets. Again, this acts as collaboration opportunity to plan and implement improvements to the EESSI services.

2.3 Cross-cutting collaboration

2.3.1 Collaboration objectives

Cross-cutting collaboration efforts will be anchored on the following common objectives.

Advancing HPC Technologies:

- Collaboratively developing and refining high-performance computing technologies to push the boundaries of computation and data analysis.
- Coordinate and strengthen the CoE initiative at pan-European level.
- Maximize impact on the European High Performance Computing HPC and user base.

Knowledge Dissemination:

- Sharing research findings, methodologies, and tools to contribute to the wider scientific community and promote open science practices.
- Strengthen the EuroHPC landscape and provide optimal support to the group of users who rely on these key technologies.
- Support collaboration, knowledge sharing and dissemination of best practices.

2.3.2 Collaboration activities

The technical and scientific partners clearly have many engineered opportunities for collaboration, but we also need to ensure that expertise also flows *between* these groups. This is ensured in a number of ways:

- The scientific application developers will include their applications and workflows within EESSI, the workflow required to enable this demands collaboration between the application developers and the technical team. For example, such a process has already taken place for ESPResSo.

- For *marquee* applications provided by the scientific partners, we also require that they help develop tests (which are run regularly), to ensure EESSI delivers applications with the expected correctness, scalability and performance levels.
- When it comes to their own applications, it is expected that the scientific partners wil also contribute to the user support services offered by MultiXscale.
- EESSI has also put CI services in place to support application developers. The technical teams will work with the application developers to enable them to leverage these services during their development processes.
- **Dissemination is a critical and shared responsibility** among all partners. We are developing an "elevator pitch" presentation of MultiXscale to give all project partners a engaging, quick but comprehensive set of presentation materials that they can use to briefly present MultiXscale at any relevant activity they participate in.

From a dissemination perspective, there are many shared activities that will be undertaken:

- Regular Virtual Meetings and Workshops: Scheduled interactions to maintain active communication and foster collaboration.
- Collaborative Publications: Co-authoring papers and publications to showcase collective research achievements.
- Community Engagement: Participating in events and outreach activities to engage with individuals beyond the project.

2.4 Collaboration with associated partners

2.4.1 Collaboration objectives

The associated partners have specific roles related to particular pilots of MultiXscale as outlined in the project DoA.

As the project matures, MultiXscale may widen the scope of what is meant by "Associated Partner" beyond the strict legal meaning within the DoA. We do expect to engage in specific and targeted collaborations with specific entities and would like to have a means of recognising the contributions of these entities to the MultiXscale objectives.

2.4.2 Collaboration activities

MultiXscale recognizes the value of engaging with **associated partners and supporters** with academic institutions and research organizations to foster knowledge exchange and access complementary expertise. Current engagements are:

- **UNIVERSITE PAUL SABATIER TOULOUSE III** with expertise in the multiscale modeling of supercapacitors, with an emphasis on lattice-based methods.
- **Max-Planck-institute** with algorithmic expertise in the coupling of lattice-Boltzmann and molecular dynamics simulations as well as the thermalization of the lattice-Boltzmann method.

With an expanded definition of "Associated Partner", we foresee additional activities:

- Direct collaboration with external community application developers to allow them to leverage the development infrastructure that EESSI provides, as well as to use it as a delivery mechanism for their software releases
- Collaboration with a wide spectrum of HPC providers to allow them to offer EESSI as an alternate (or indeed primary) software stack on their systems.
- Collaboration with community scientists them to enable to ship their workflows along with EESSI so that they can be used by others.

3 Collaboration with EuroHPC Ecosystem

The origins of MultiXscale is rooted in HPC ecosystem collaboration. It stands as a pioneering example of resource federation, bringing together highly skilled technical personnel from Tier 0, 1, and 2 HPC centers through the EESSI initiative, and complementing this expertise with the algorithmic and scientific proficiencies of the CECAM network.

MultiXscale has established, robust connections and collaborations with partners from legacy projects such as **PRACE, CASTIEL, and Fenix-RI**, **inheriting the legacy of E-CAM**. Furthermore, it counts among its partners several **actively engaged in ongoing EuroHPC infrastructure projects and National HPC Competence Centers**.

3.1 Ambassador program

3.1.1 Collaboration objectives

Ambassador Development:

- Nurturing the next generation of HPC experts through training, mentor-ship, and educational outreach initiatives.
- Facilitate and guide the raising of standards of competence in the provision of HPC and related technologies to academia, public administration and industry.

3.1.2 Collaboration activities

MultiXscale's commitment extends to continuing the **fruitful partnerships initiated by E-CAM with other HPC CoEs**, particularly in **application development and training endeavors**. The creation of an **"Ambassador Program"** for CECAM nodes and NCCs is in progress, with the objective of reaching and supporting user communities across all EuroHPC countries and beyond, as part of WP6.

The application co-design for exascale objective of the project provides advice and direction for users on how to prepare for exascale (WP6) and gives them the tools to do so (WPs 1-5). Our approach to software delivery ensures that even researchers in "EU countries currently developing and advancing their HPC infrastructure" can benefit from the CoE's advancements, irrespective of national facilities.

3.2 Collaboration with CASTIEL2

3.2.1 Collaboration objectives

The mission of **CASTIEL 2** encompasses the **harmonization and reinforcement of endeavours undertaken by the NCC and CoE initiatives on a pan-European scale**. Its primary goal is to **facilitate collaboration** among NCCs and CoEs, fostering their influence on European High-Performance Computing (HPC) and its user base. CASTIEL 2 aims to consolidate the collective influence of CoEs and NCCs by **nurturing networks, promoting interaction, and addressing disparities** in HPC expertise across countries. It will also enhance the EuroCC Access portal to serve as a comprehensive reference point for European HPC expertise, software, training resources, events, and services. CASTIEL 2's objective is to elevate competency standards in HPC provision to academia, public administration, and industry, and it establishes itself as a reference entity for CoEs and NCCs, encouraging collaboration, knowledge exchange, and best practices dissemination. Through the **collaboration of CoEs and NCCs, CASTIEL 2 aims to strengthen the EuroHPC landscape** and provide robust support to the user groups dependent on these essential technologies.

3.2.2 Collaboration activities

MultiXscale participates actively in various activities outlined across CASTIEL 2 work packages. These activities are spread across CASTIEL 2:

- In WP2 "NCC/CoE Networking and Competence, Code, and Service Mapping", CoEs will work on summarizing information about themselves, contribute to task forces on specific topics of interest, and provide expertise, collect requirements from CoEs and end-users on competence mapping, codes, and services;
- In WP3 "Training, Twinning, and Mentoring", CoE training champions will interact with NCC training champions, and joint training courses will be organized, task forces for training-related collaborations and material exchange will be established;
- In WP4 "NCCs, CoEs, and Industry Interactions", CoE industry champions will engage with NCC industry champions, producing a summary document about CoEs regarding industry-related topics; regular meetings will be

held to share updates and knowledge; CoEs will also participate in events organized by CASTIEL 2 to enhance industry knowledge sharing;

- In WP5 "Awareness, Impact, and Outreach", the communication strategy will highlight CoEs' activities and success stories, including the expansion of the EuroCC Access portal to encompass CoEs and other entities. The WP will provide support for CoEs' communication efforts and coordinate continuous integration with CoEs for codes to be available on European High Performance Computing Joint Undertaking (EuroHPC JU) Systems.

Internally, within **MultiXscale**, we have determined **champions** who are responsible for each of the WP:

- **CASTIEL 2 WP2 - Networking and Competence champions** - Matej Praprotnik (National Institute of Chemistry (NIC)) and Ignacio Pagonabarraga (University of Barcelona (UB))
- **CASTIEL 2 WP3 - Training champion** - Alan O'Cais (UB)
- **CASTIEL 2 WP4 - Industry champions** - Antonio Scirappa and Carlo Cavazzoni (both LEONARDO)
- **CASTIEL 2 WP5 - Communication champion** - Elisabeth Ortega and Susana Hernandez (both HPCNow!)

CoEs will collaborate not only with CASTIEL 2 but also among themselves, with CASTIEL 2 facilitating this collaboration. CoEs will engage in the Competence Centre and CoEs Advisory Board, join working groups, and participate in joint events.

MultiXscale collaboration within the CASTIEL 2 ecosystem entails sharing a lot of information between CASTIEL2 and the CoEs, including:

- CAB Meetings: Invitations, minutes and any further material
- Invitation to participate in the organization of events
- Competence and Services Map
- Training activities: sharing of training-related goals and best practice guides, available training-related resources and training materials/documents
- HPC in Europe Portal: Information about the CoEs training events, ideally shared in the training registry (HPC in Europe portal)
- Deliverables: For all CASTIEL 2 deliverables, where input of the CoEs is needed according to the DoA
- Access to the CoEs DoAs: apart from information falling under a strict confidentiality clause
- Industry interaction: Data on industry interaction (Small and midsize enterprise (SME)s and Large industry) of the CoEs will be collected (if not confidential)
- Communication: Exchange of expertise and resources with regard to communication work
- Minutes and slides

Active contributions of MultiXscale to the associated Coordination and support action of CASTIEL2 include (or will include):

- Contribution to the knowledge pool and available information to the common portal C2ISS
- Establishing effective collaborations and jointly addressing cross-cutting issues
- Participating in regular meetings to plan, implement and monitor collaborations and to synchronize research and development activities
- Actively contributing supported codes and in the common continuous integration and application deployment platform with automated testing (e.g., using Special Access scheme in collaboration with CASTIEL 2) at least on all EuroHPC JU systems
- Establishing common best practices for IP management and development including effective measures to ensure code quality, reviews, testing, management and development cycles
- Actively advancing modularisation: implementation of concrete measures for identification of common routines/algorithms/modules, creation and extension of software libraries used by multiple codes across disciplines
- Participating in benchmarking exercises
- Sharing results and best practices as relevant
- Joint publication and dissemination of results

- Participation on joint events
  - Training Champions Meetings & Workshops
  - Industry Code of the Month: CoEs have the opportunity to present their industry services and potential collaborations through an "Industry Code of the Month" event.
  - Workshop Series for Code & Service Promotion
  - Industry Sector Events: CoEs and NCCs jointly attend industry sector-specific events to showcase their service offerings.
  - Thematic Webinars: Webinars are organized to promote specific codes and applications from multiple CoEs
  - WP 4-CoE Meetings: WP 4 organizes meetings every three months for CoEs and industry representatives to share updates, knowledge, and requests.
  - Industry Coffee Breaks: These facilitate focused exchanges among industry specialists.
  - Communication Coffee Breaks: Similar to the industry coffee breaks, these enable discussions among communication specialists.
  - Communication Champion Meetings: Small group meetings with CoE Communication Champions promote collaboration and exchange on current topics.
  - Joint Workshops with NCCs: General workshops or conferences may be organized during the project to bring together domain experts from CoEs and the National Competence Centers.

3.3 Collaboration with industry

While industrial collaboration is not a critical aspect of MultiXscale, there are clear existing collaboration activities that are both substantial in size, and with significant scope for future growth.

3.3.1 Collaboration objectives

- Advertise and facilitate the adoption of the solutions provided by MultiXscale among industrial communities.
- Make it easier for industrial users to adapt to new archtitectures (with a keen eye on future adoption of RISC-V solutions).
- Create tools and workflows that allow the adoption and utilisation of EESSI in cloud environments.

3.3.2 Collaboration activities

With the participation of two industrial partners, Leonardo and HPCnow!, there are clear use cases for the scientific aspects of MultiXscale (helicoptor design and certification for Leonardo) and the technical solutions EESSI is developing (for application delivery to customers of HPCnow!).

In addition, EESSI receives substantial in-kind support from both Azure and AWS to support the development of the platform. The practical motivation for this support from their perspective is clear: EESSI is a game-changing initiative for application support within cloud environments. EESSI provides a consistent user experience irrespective of the underlying architecture technology, and without the need for them to directly support their scientific user community for community codes. It also provides a stable platform upon which they can provide additional application solutions.

4 Conclusions

When creating the consortium for MultiXscale, significant consideration was given to the capacity for the development of mutually beneficial collaborations. These collaborations extend beyond the obvious scientific and technical components of the project, but ensure that both these components provide input and feedback that can be leveraged by the other group. The internal collaboration activities described in this deliverable are therefore extensive, ranging from low to high levels of detail and maturity in implementation.

As regards external collaboration, in the initial year of MultiXscale this is dominated by the collaboration with CASTIEL 2, with whom a Collaboration Agreement (CA) is currently being drawn up. A number of activities detailed in the CA are reproduced to some extent in this document in order to make it self-contained.

Beyond CASTIEL 2, MultiXscale has interest in generating collaborations with additional scientists in the CECAM community, and also with industry. The CECAM network represents a significant portion of the target community of MultiXscale, so the motivation there is clear. For industry, initial concern is retaining the support of large cloud providers who currently provide substantial cloud credits to EESSI so that it can deliver the services it does.

References

Acronyms Used

HPC High Performance Computing
CECAM Centre Européen de Calcul Atomique et Moléculaire
WP Work Package
CoE Center of Excellence
EESSI European Environment for Scientific Software Installations
NIC National Institute of Chemistry
EuroHPC The European High-Performance Computing
ESPResSo Extensible Simulation Package for Research on Soft Matter
C2ISS Cloud Cyber Intelligent Security Software
waLBerla widely applicable lattice Boltzmann from Erlangen
LAMMPS Large-scale Atomic/Molecular Massively Parallel Simulator
NCC National Competence Centre for High Performance Computing
NIC National Institute of Chemistry
UB University of Barcelona
EuroHPC JU European High Performance Computing Joint Undertaking
DoA Description of the action
SME Small and midsize enterprise
CI Continuous Integration
CA Collaboration Agreement

URLs referenced

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