D7.1

Collaboration plan with definition of common objectives and activities including milestones

Luisa Neri, Nicola Spallanzani, Andrea Ferretti

Due date of deliverable: 30/06/2023 (month 6)
Actual submission date: 30/06/2023
Final version: 30/06/2023

Lead beneficiary: CNR (participant number 1)
Dissemination level: PU - Public

Document information

Project acronym:	MAX
Project full title:	Materials Design at the Exascale
Research Action Project type:	Centres of Excellence for HPC Applications
EC Grant agreement no.:	101093374
Project starting / end date:	01/01/2023 (month 1) / 31/12/2026 (month 48)
Website:	www.max-centre.eu
Deliverable No.:	D7.1

Authors: Luisa Neri, Nicola Spallanzani, Andrea Ferretti

To be cited as: L. Neri, N. Spallanzani, A. Ferretti, (2023): Collaboration plan with definition of common objectives and activities including milestones. Deliverable D7.1 of the HORIZON-EUROHPC-JU-2021-COE-01 project MAX (final version as of 23/06/2023). EC grant agreement no: 101093374, CNR, Consiglio Nazionale delle Ricerche, Italy.

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Executive Summary

MAX - MAterials design at the eXascale (GA 101093374) is a Centre of excellence for HPC applications funded in the joint EuroHPC-Horizon Europe call. It develops and uses its lighthouse (quantum simulation) codes[1] to enhance the understanding, predicting, and discovering of the properties and performance of materials, to address the HPC-ecosystem challenges, to leverage the opportunities arising from future exascale and post-exascale architectures, and to offer powerful paths to discovery and innovation serving both scientific and industrial applications.

In this endeavour, MaX will collaborate with the complementary projects and the dedicated Coordination and Support Action (CSA) CASTIEL 2 (Grant No 101102047) by developing the following activities:

- Actively contributing to the coordination activities of CASTIEL 2
- Contributing to the knowledge pool and available information in 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 synchronise research and development activities
- Participating in benchmarking exercises
- Sharing results and best practices as relevant
- Joint publication and dissemination of results
- Joint events
- Actively contributing supported lighthouse codes to a 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, provided that a suitable IT infrastructure and access agreements are put in place by EuroHPC JU

[1] QUANTUM ESPRESSO, Yambo, Siesta, Fleur, BigDFT.

- 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.

This deliverable shows how, at Month 6, we plan to implement these activities.

1. Introduction

The MAX - Materials design at the exascale CoE has been funded under the EuroHPC JU Call HORIZON-EUROPEHPC-JU-2021-COE-01, which has among its main goals a continuous collaboration among the CoEs funded in the same call (hence, complementary CoEs) and the relevant Coordinating and Supporting Action CASTIEL 2.

The overall goals for this activity are the definition of common objectives and synergic strategies and have been described in the GA in T7.3 *Common activity for complementary grants* (Collaboration task) (months 1-48, Task leader: E. Molinari – CNR, Partners: All) as follows:

- Actively contribute to the coordination activities of the associated CSA
- 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 synchronise research and development activities
- Participating in benchmarking exercises
- Sharing results and best practices as relevant
- Joint publication and dissemination of results
- Joint events
- Actively contributing supported lighthouse codes to a common continuous integration and application deployment platform with automated testing (e.g., using a Special Access scheme in collaboration with CASTIEL 2) at least on all EuroHPC JU systems, provided that a suitable IT infrastructure and access agreements are put in place by EuroHPC JU.
- 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

The collaboration between MAX (and the complementary CoEs) and CASTIEL 2 will be formalised and described by several documents:

1) The CSA's and CoE's Grant Agreements that describe mechanisms and goals for collaboration;
2) The Collaboration Agreement due at M6 that regulates legal aspects, including confidentiality, access rights for use, GDPR issues, etc.

To monitor the advancement of these activities, four key performance indicators (KPIs) have been added to the MAX list of KPIs:

KPI	DESCRIPTION
K3.4	No. of applications deployed to JU systems incl. breakdown by partition (e.g. CPU, GPU).
K3.5	No. of EUROHPC systems supported by application incl. breakdown by partition (e.g. CPU, GPU).
K3.6	No. of errors (failed deployments/ regression tests) identified through common platforms.
K3.7	Average time from failed application test to deployment of corrected application.

Table 1. Collaboration KPIs from DoA

In this deliverable, we will describe the actions undertaken and foreseen in establishing a collaboration with the CSA, the National Competence Centres, and the complementary Centres of Excellence, in order to systemize expertise and knowledge for the enhancement of HPC applications in Europe.

2. Establishing a collaboration with the CSA

The first action listed in T7.3 builds the framework for all other actions, and a lot of effort has been put by all our Work Packages in order to be actively and fruitfully involved. The action requires to **Actively contribute to the coordination activities of the associated CSA.**

CASTIEL-2 (01/2023-12/2025) is the CSA supporting HPC E-CoEs and NCCs successor to both CASTIEL (NCCs) and FocusCoE (CoEs) (Grant No. 101102047) that has the role of providing coordination support to the EuroHPC CoEs an NCCs. It aims at building a stronger HPC community which will foster strategic collaboration in HPC research and deployment of skills and in expertise in HPC technologies and applications between CoEs and NCCs.

MAX played a key role in the activities of FocusCoE (2018-2022), profiting from the development of common actions, of interactions with other CoEs, support in sustainability, communication, training and more activities. In this framework, we are glad to tightly collaborate with CASTIEL 2 in structuring the common HPC ecosystem and boosting the single NCCs and COEs results, outcomes, outputs by building a rich network and systematising competences.

To begin with, we appointed a list of Champions and Deputies to attend the CASTIEL 2 activities organised by their work packages (February 2023).

WP	Champion	Deputy
WP2 NCC/CoE networking and mapping of competences, codes and services	Nicola Spallanzani (CNR)	Andrea Ferretti (CNR)
WP3 Training, Twinning Mentoring	Daniele Varsano (CNR)	Maria Bartolacelli (CNR)
WP4 NCCs, COEs and industry interaction	Luisa Neri (CNR)	Nicola Spallanzani (CNR)
WP5 Awareness, impact, outreach & sustainability	Àlex Argemí (ICN2)	Virginia Greco (ICN2)

Table 2. MAX reference personnel for CASTIEL 2

We have since attended all CASTIEL 2 meetings:

- Kick-off in Stuttgart, DE on February 8 and 9, 2023. Nicola Spallanzani (CNR) attended in person to introduce MAX and many others from MAX participated online;

- NCCs-CoEs meeting, April 18-19, 2023 online. Nicola Spallanzani (CNR) presented MAX to other participants. Other MAX people attended the thematic rooms on industry, training, and communication.

Plan: we are willing to continue to attend the CASTIEL 2 meetings and to participate in thematic meetings, collaborating and contributing to all requests.

3. Technical deployment

CI/CD Platform

Continuous Integration and Continuous Deployment (CI/CD) practices have become increasingly relevant in the context of High-Performance Computing (HPC), where code integrity, performance optimization, and efficient deployment are paramount. HPC codes often involve complex software stacks, parallel processing, and dependencies specific to different hardware architectures. CI/CD for HPC codes aims to automate the build, testing, and deployment processes to ensure code correctness, performance, and compatibility across diverse HPC environments. Automating the build process using build automation tools (e.g., Spack, EasyBuild, etc.) allows for consistent and reproducible builds across different environments. Automated builds ensure that all necessary dependencies are correctly resolved and that the code can be compiled without manual intervention.

In order to facilitate the deployment of CoE codes on all the EuroHPC supercomputers, CASTIEL 2 is driving the implementation of a unified CI/CD platform. Since every HPC centre is already providing a CI/CD procedure for its users, CASTIEL 2 decided to pair the HPC centres with one or more CoEs in order to start some tests. Based on these preliminary tests CASTIEL 2 will collect all the desiderata and will develop the platform in collaboration with all the stakeholders.

Pairing a CoE with a EuroHPC hosting should allow both sides to learn from each other. On the one hand, a CoE shall get some hands-on experience with the existing CI/CD environment at a selected hosting site. On the other hand, a hosting site can get insights into specific requirements imposed by codes from the CoE. For this, we would like to allow all involved persons to explore CI/CD for the first four to five weeks of work. Ultimately, CASTIEL 2 would

like to ask each CoE during the regular CI/CD dedicated calls to report on their experience, ideally with a few presentation slides for guidance.

CASTIEL 2 paired the MaX CoE and ESiWACE CoE with the CINECA supercomputing centre in order to start this collaboration.

Within the scope of MAX T3.4 *Deployment on EuroHPC machines,* we embraced the CASTIEL 2 initiative following all the organised meetings on the topic and starting the collaboration with the HPC centre paired with our CoE. Indeed, the goal of this task is the effective deployment and tuning of the MAX lighthouse codes and workflows on EuroHPC systems. This work will include the support to the runs for the workflows inspired by the scientific grand challenges and their optimisation. This includes also the production of environment modules and container-based solutions for the HPC deployment of MAX applications. This task will also contribute to the execution of benchmarks, reporting the results in terms of the efficiency, on the EuroHPC systems.

Moreover, the consolidation of the recipes for automation tools like Spack or EasyBuild for all the MAX codes is crucial for establishing standardised and reliable software management practices in CI/CD, ensuring consistency, reproducibility, and streamlined deployment of the codes across diverse HPC environments.

Special Access Scheme

CASTIEL 2 supports the CoEs programs in gaining appropriate access to EuroHPC supercomputers to meet their deployment and delivery objectives. To facilitate this, CASTIEL 2 conducted surveys to gather initial requirements from CoEs and compiled a detailed proposal for a special access scheme. The CoEs plan to deploy approximately 60 codes and pilots on EuroHPC supercomputers, but there is uncertainty regarding resource requirements and compatibility. To address this, CASTIEL 2 proposed to the EuroHPC JU two initial access models: a flat-rate approach for benchmarking and development, and an individualised yet accelerated approach for regular and high-priority access. Additionally, CASTIEL 2 recommends implementing a process for resource estimation updates and periodic checks on resource usage to allow for adjustments as needed. MAX CoE developers will continue to contribute providing feedback and suggestions.

4. Collaboration between MAX and CASTIEL 2, and CoEs/ NCCs

Being MAX active since 2015, it has established a long and stable collaboration network with other CoEs, regarding technical deployment, training and dissemination activities, and exchange of good practices. As envisaged by CASTIEL 2, MAX actively takes part in the life of HPC CoE Council (HPC3) since its foundation, and will continue to do so, providing advice, contributes when relevant. The same effort will be done in participating in actions promoted and organised by EuroHPC JU (as, e.g., the participation to the common booth at ISC 23).

Enabling Exchange of Expertise

One of the main features of MAX is to provide training for users, developers, researchers, students of its lighthouse codes and it has a well-grounded tradition in this field, developed by exploiting in a systematic and coordinated way the single training actions organised by its partners. Schools, hackathons, research in lab experiences, and participation as teachers and mentors to third-party events are coordinated by WP5 *Training & Community engagement within the HPC ecosystem*, led by Daniele Varsano (CNR). T5.3 regards the *Coordination and contribution to transverse training initiatives*, along the whole life of the CoE. This task involves MAX coordination and contributions to transverse training initiatives across different domains within the European HPC ecosystem through its domain-specific content. MAX will actively participate in designing, structuring, and implementing these initiatives, collaborating with various stakeholders such as National Competence Centres, HPC centres, other CoEs, and EuroHPC Training Activities and EuroHPC Professional Traineeships funded by Digital Europe Programme.

The focus is on domain-specific content, software development know-how for exascale systems, and the integration of new knowledge into university education. The following activities will be undertaken:

- **Contribution to Courses and Training Initiatives with National Competence Centres**: MAX will provide domain-specific content and expertise on software development for exascale systems and beyond. This contribution will enrich the training activities coordinated with National Competence Centres.

- **Contribution to Courses and Training Initiatives with HPC Centres, and other CoEs**: MAX will actively participate in training initiatives organised by HPC centres, the EuroHPC JU training platform and other CoEs. This collaboration will ensure the integration of MAX domain-specific knowledge and expertise into broader training programs.
- **Contribution to Training Portals**: MAX will contribute to the training portals of National Competence Centres and joint portals within the European HPC ecosystem. This contribution will include providing an events calendar and access to online training materials, such as the HPC in Europe portal.
- **Contribution to CASTIEL 2 CSA training activities**: MAX will actively promote and participate in events coordinated and promoted by the CSA CASTIEL 2, by providing domain specific content and sharing its experience in delivering training in networking events as, e.g., Virtual Training coffee breaks.
- **Development of Flexible Teaching Modules**: MAX recognizes the importance of integrating new knowledge into university education. Flexible teaching modules based on MAX lighthouse codes will be developed and tested. These modules will target Master's/Ph.D. students and university professors interested in frontier computational methods within their respective disciplines, such as computational materials science, computational physics, computational chemistry, etc. Collaborations with institutions hosting existing Master's or Ph.D. courses based on HPC will be fostered, and collaborations with the European Master for High Performance Computing (EUMaster4HPC) will be pursued on selected teaching modules based on MAX lighthouse codes.

The outputs of this task will include contributions to training initiatives coordinated with National Competence Centres and the wider European HPC ecosystem. Additionally, teaching modules will be developed for adoption in Master's/Ph.D. courses, ensuring the systematic dissemination of frontier computational methods and the utilisation of MAX lighthouse codes in educational settings.

A fruitful collaboration was established with ENCCS, the EuroCC National Competence Center Sweden, that has already led to the co-organization of a 3-day School[2] on “Efficient materials modelling on HPC with Quantum ESPRESSO, Yambo and BigDFT" from 14 to 17 November 2022. All the training material is available on-line. On June 12, 2023 Nicola Spallanzani (CNR) gave a

[2] https://enccs.se/news/2022/12/efficient-materials-modelling-workshop/

talk at the MPI/OpenMP course, organised by NCC Netherlands with PRACE and HLRS: he introduced MAX and its lighthouse code applications, before going deeply in details about algorithmic design and implementations[3].

Fostering Industrial Interaction

Being MAX a CoE funded by HORIZON-EUROHPC-JU-2021-COE-01, it does not have industrial uptake as one of its core tasks. Nonetheless, we consider it very important to increase and extend engagements with established and potential industrial end-users. Potential industrial users of the lighthouse codes are therefore a key target community for our communication and dissemination activities, and a crucial potential actor for exploitation of MAX results. Additionally, hardware (HW) manufacturers and software (SW) vendors are important actors, both in the co-design activities and in the potential for economic impact of the MAX applications if incorporated into commercial services and products. Interaction with relevant HW manufacturers is ensured due to their participation in the consortium, and the links already established with external ones (e.g., NVIDIA, IBM). Links with SW vendors, as possible exploitation channels for MAX software developments, will focus on companies within the European Union and the Participating States of the EuroHPC Joint Undertaking.

Therefore, we plan to actively attend and contribute to most of the activities promoted by CASTIEL 2 in its WP4 *NCCS, COEs AND INDUSTRY INTERACTION*, from surveys to webinar to sectorial events, and more. To begin with we intend to present in the next months our codes to the CASTIEL 2 Code-of-the-month webinar series.

Communication support

MAX has a rich portfolio of communication tools to promote and disseminate its actions and has always considered it very important to promote and disseminate those of the HPC/ domain ecosystems. Besides dissemination activities such as participation in conferences, events, training initiatives, MAX runs a website[4], a Twitter account[5], a LinkedIn page[6], and a YouTube

[3] https://eurocc-netherlands.nl/calendar/mpi-and-openmp-in-scientific-software-development/
[4] www.max-centre.eu
[5] https://twitter.com/max_center2
[6] https://www.linkedin.com/company/max-centre

channel[7]. These activities are led by WP6 *Communication, exploitation, and dissemination*, coordinated by Àlex Argemí (ICN2), in full collaboration, also for activities regarding this Collaboration Plan, with WP5 Training and WP7 Management.

Interaction with supercomputers and NCCs is crucial for MAX, as they are key actors in dissemination of our results and products, the engagement of the user's communities, and training events, schools and hackathons organised by and around MAX. They will be both a target of our communication and dissemination activities, and sources of information about MAX to the HPC community at large. Direct channels of communication will be established through the management team with the different NCCs (including those already present in MAX as partners of the consortium, like BSC in Spain and Leonardo and CINECA in Italy).

5. Outlook & Next Steps

The collaboration of MAX with the CSA and other CoEs/NCCs set in the Grant Agreement has started to work. MAX will continue to play its role both in the technical deployment and in the training, exploitation, communication activities, making its best to be paramount in building the European HPC ecosystem and reaching the targets aiming to improve the whole community.

Next steps:

- **Collaboration agreement**: due at M6 as from the specific milestone M7, it is undergoing review under the responsibility of the CSA and will be available soon.

Milestones

Grant Preparation (Milestones screen) — Enter the info.

Milestone No	Milestone Name	Work Package No	Lead Beneficiary	Means of Verification	Due Date (month)
7	Collaboration agreement has been signed.	WP7	1-CNR	Collaboration agreement with CSA Castiel 2 is signed.	6

Fig 1. Milestone 7 definition from MAX DoA

- **Definition of common KPIs.** targets for collaboration-related KPIs (K3.4, K3.5, K3.6, K3.7) are under definition. They are due within month 12 according to MAX DoA and will be shared with the CSA as soon as they are ready.

[7] https://www.youtube.com/channel/UCcoGe0aUy4gDVRNgjQlVf3g

- **Deliverables**. Four deliverables about the collaboration activities are planned for MAX. The next deliverables will update on the available applications and different versions deployed via the common platform and report the common activities performed in all WPs.

Deliv. no.	Deliverable Title	Lead beneficiary	Month	Status
D7.1	Collaboration plan with definition of common objectives and activities including milestones	CNR	6	done
D7.4	Update of collaboration plan	IJS	12	
D7.6	Second update of collaboration plan	BSC	30	
D7.9	Final report of collaboration plan	BSC	48	

Table 3. List of MAX deliverables on Collaboration with CSA and CoEs and NCCs