



Deliverable D7.4: Update of collaboration plan (month 12)

## D7.4

### Update of collaboration plan (month 12)

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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 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. MAX involves active developers of the codes, researchers that are expanding and innovating in the algorithms and models as well as software engineers and support personnel for dissemination, training, code review and benchmarking, to provide a complete ecosystem as needed to achieve the scalability and reliability required by the challenges of the HPC-ecosystem evolution.

In this endeavour, MaX will continue to collaborate with the complementary projects and the dedicated Coordination and Support Action (CSA), CASTIEL 2 (Grant No 101102047), by developing common scientific activities, joint training and communication actions.

Importantly, MaX will continue to play an active and leading role toward the optimal deployment and performance of codes on the EuroHPC machines, according to the plans and joint commitments that are being finalised with the coordination of CASTIEL 2.

This deliverable provides an update and critical review of the work performed at Month 12, essentially confirming the initial plan (D 7.1, Month 6) and allowing for a more detailed definition of the implementation strategies.

### 1. Introduction

The MAX - Materials design at the exascale Centre of Excellence (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:

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- Active contribution to the coordination activities of CASTIEL 2;
- Contribution to the knowledge pool and available information in the common portal C2ISS;
- Establishment of effective collaborations and jointly addressing cross-cutting issues with CSA and the actions the CSA coordinates with;
- Participation in regular meetings to plan, implement and monitor collaborations and to synchronise research and development activities;
- Participation in joint deployment and benchmarking exercises;
- Sharing results and best practices as relevant to CSA's supported activities and communities;
- Joint publication and dissemination of results;
- Participation in joint events;
- Active contribution of 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, using technical access accounts or approved benchmarking access) at least on all EuroHPC JU systems, provided that a suitable IT infrastructure and access agreements are put in place by EuroHPC JU;
- Establishment of common best practices for IP management and development including effective measures to ensure code quality, reviews, testing, management and development cycles;
- Providing feedback for consideration of security best practices in code quality, review, testing and development cycles (as a new measure to safe-guard the future joint technical efforts);
- Active advancement of modularisation: implementation of measures for identification of common routines/algorithms/modules, creation and extension of software libraries used by multiple codes across disciplines.

The collaboration between MAX (and the complementary CoEs) and CASTIEL 2 has been 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 but delayed towards M16– that regulates legal aspects, including confidentiality, access rights for use, GDPR issues, etc.

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

KPI	DESCRIPTION
K3.4	No. of applications deployed to JU systems including breakdown by partition (e.g. CPU, GPU).
K3.5	No. of EUROHPC systems supported by application including 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.

As proposed, the same format of KPI has been picked up by CASTIEL 2 to monitor progress and we have started to report on the current status for CASTIEL 2 to be able to gather the status from all contributing CoEs.

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

## 2. Establishing the 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 and to communicate the joint activities to all the partners and coordinate the project evolution. 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 and NCCs. It aims at building a stronger HPC

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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.
- Since May 2023, regular CASTIEL 2 meetings for CI/CD coordination with CoEs and deployment have been held and attended by MAX representatives.
- MAX representatives attended the different regular meetings of WP3 “Training, Twinning Mentoring”, WP4 “NCCs, COEs and industry interaction” and WP5 “Awareness, impact, outreach & sustainability”.



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Below a list of attended meetings and activities performed in the framework of the 3 different CASTIEL 2 WPs.

**WP3 Training, Twinning Mentoring COFFEE BREAKS** (monthly meeting on the first Thursday of the month, starting from May 2023)

- 04/05/2023
- 01/06/2023
- 06/07/2023
- 07/09/2023
- 05/10/2023: Daniele Varsano (MAX WP5 Leader “Training and Community Engagement within the HPC ecosystem”) presented MAX training - past, present and future activities and collaborations;
- 02/11/2023
- 30/11/2023 special meeting: Daniele Varsano (WP5 Leader) and Luisa Neri (WP7 Leader) with the new CASTIEL2 WP Leader Aline Melinette;
- 07/12/2023

**WP4 NCCs, COEs and industry interaction COFFEE BREAKS** (monthly meeting on the fourth Thursday of the month, starting from September 2023)

- 28/09/2023
- 26/10/2023
- 23/11/2023

Further collaborations with CASTIEL 2:

- **Nicola Spallanzani** for MAX took part in the Kick-off of CASTIEL2 held on February 8-9 in HLRS Stuttgart (DE). He presented MAX during the special session for the Centres of Excellence (CoE) and got in touch with the other CoEs representatives.

We will continue to attend the CASTIEL 2 meetings, to participate in thematic meetings, collaborate with NCCs and other CoEs and continue contributing feedback to all requests.

### 3. Technical deployment

#### 3.1 Advanced Technologies Monitoring

MAX has a strong focus on identifying interesting technologies that will come up in the next few years and can be used as co-design platforms, advanced hardware platforms, and systems suitable for energy-efficiency evaluation. Within this effort (WP4), we engage in contacts with HPC sites, universities and vendors in order to gain access to these platforms. They will then be

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primarily utilised for benchmarking purposes via application kernels extracted from MAX codes, but in some cases entire applications will be used to validate the software solution on an architecture.

A number of interesting architectures and novel technologies can be provided to the effort by consortium partners (i.e., ARM (A64FX) processors, Intel's 512GB NVDIMM persistent memory modules, Bittware 520N-MX FPGA cards, FPGA Xilinx Alveo U250 Data Center Accelerator Cards, Ampere Altra Q80-30, NVIDIA BlueField-2 DPU, Power 10 CPUs, ARM Neoverse-N1 80-Core CPUs, AMD MI200), but in other cases we rely on collaboration with outside entities and industrial actors. In some instances (IT4I, E4) direct access can be provided, in others (EVIDEN), case by case solutions have been arranged within MAX. We are in contact with the European pilot for exascale (EUPEX) project to gain access to Fujitsu A64FX CPUs and EUPEX software stack, expected to start operation in Q1 2024. Access to the system will be granted upon acknowledged request to the EUPEX consortium. Similarly we expect to coordinate with SiPearl to have their personnel perform runs on their development set-ups if necessary.

We expect further collaboration with vendors and developers to gain early access to new technologies for this effort.

### 3.2 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. In the development process, automating build processes on different platforms allows developers useful and regular feedback from platforms they might not have regular access to. Such feedback has become paramount to achieve compatibility and scalability due to the complexity of the HPC ecosystem, where new and complex platforms are being deployed and used regularly. 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 HPC centres are already providing a CI/CD procedure for its users, CASTIEL 2 decided to pair the HPC centres with one or

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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 and ESIWACE CoEs with the CINECA supercomputing centre in order to start this collaboration. This corresponds to our existing engagement, since Leonardo<sup>1</sup>, the pre-exascale Tier-0 EuroHPC supercomputer hosted by CINECA, had been proposed as the preferred system for the profiling and benchmarking activities within MAX WP3 (Leonardo was the largest HPC architecture available within MAX and accessible to all MAX code developers). In addition, within the CASTIEL 2 project –promoting interaction and exchange between National Competence Centres– we should soon have access to other EuroHPC architectures. Then, MAX codes will be ported and deployed on all the architectures we will have access to, addressing possible issues and working towards their resolution. Since the MAX CoE had an existing infrastructure and already used some of the participating EuroHPC hosting sites, we have decided to accelerate and expand the process by including the EuroHPC systems Vega, hosted at IZUM/SLING, and Karolina, hosted at IT4Innovations.

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 as well as the supporting centre. Indeed, the goal of this task is the effective deployment and tuning of the MAX lighthouse codes and workflows on EuroHPC systems. This work includes supporting execution of workflow inspired by the scientific grand challenges and their optimisation. We have envisaged to include the production of environment modules and container-based solutions for HPC deployment of MAX applications. To support this effort, our members are participating in EuroHPC HPC Container Forum (regular monthly regular meetings, including an in-person meeting at the EuroHPC Summit 2023).

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<sup>1</sup> <https://www.hpc.cineca.it/systems/hardware/leonardo>

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For the benchmarking effort within MAX we adopted JUBE<sup>2</sup>, a tool developed at the Julich Supercomputing Center that provides a script-based framework to easily create benchmark sets, run them on different computer systems and evaluate the results. We are promoting the use of JUBE as “the agnostic benchmarking system” in interactions with other CoEs and within CASTIEL 2 meetings in order to make the exchange of information and results easier in the future. CINECA organised a webinar dedicated to JUBE followed by a mini-hackathon. The webinar documentation with related examples are available in the JUBE4MAX<sup>3</sup> repository, dedicated to MAX JUBE material and can serve as an example for setting up HPC benchmarking for advanced codes on multiple architectures.

In our exchanges with CASTIEL and the other CoEs, we contacted MultiXscale which promotes CVMFS distributed storage system as the solution to provide software on all EuroHPC clusters, which could be a good fit for optimised software distribution for all CoEs. Our CI/CD team is in favour of this proposal to be used for MAX and supports CASTIEL 2, within their coordination efforts, to find a way to have the EuroHPC hosting sites support this solution. The minimal effort required from the hosting sites (installing a squid server as a caching solution to enable faster software utilisation and installing cvmfs-clients on the worker nodes) could facilitate centralised / orchestrated software deployment and would profit from the fact that CVMFS is suitable also for small files, which makes the use of sandboxed software containers using CVMF easy, straightforward and efficient. The solution is already supported on Vega and Karolina.

This task will also contribute to the execution of benchmarks, reporting the results in terms of the performance efficiency as well as power efficiency, on the EuroHPC systems.

Moreover, the consolidation of the recipes for automation tools like Spack or EasyBuild for all the MAXcodes 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.

### 3.3 Special Access Scheme

CASTIEL 2 committed to support 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

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<sup>2</sup><https://www.fz-juelich.de/en/ias/jsc/services/user-support/software-tools/jube?expand=translations,fzisettings,nearrest-institut>

<sup>3</sup>[https://gitlab.com/max-centre/JUBE4MaX/-/tree/develop?ref\\_type=heads](https://gitlab.com/max-centre/JUBE4MaX/-/tree/develop?ref_type=heads)

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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 developers continue to contribute and provide feedback and suggestions. We have proposed a structured technical support mode to allow CI/CD processes to run with dedicated identities and with suitable access modes and we started to address the minimal security, authentication and authorization requirements.

We have experimented on two EuroHPC sites, Karolina and Vega, to prepare an assessment of efficiency, ease of use and security implications of technical access as opposed to standard project access within the special access scheme. The SSH executor, while working and producing results, has not been accepted as a good solution. Our CI/CD group suggests using dedicated users, in our case GitLab runner with Jacamar (providing shell and SLURM executor), which requires technical access on site with the relevant support. In this case, Jacamar-auth is used for authorisation controls, which enables isolation between CI jobs on the runner host. We expect that different authentication and 2FA solutions together with different supported methods for GitLab runners on sites will be a barrier to uncomplicated implementation of a unified solution by CASTIEL 2 and might require CoEs to provide different solutions for each site. We suggest that a unified/independent solution should be provided that requires no support from the individual hosting entity. We have established this discussion within CASTIEL 2 and intend to work with the other CoEs towards a common resolution.

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

MAX is a well established CoE, active in successive editions since 2015. As such, it has a well established collaboration network with other CoEs regarding technical deployment, training and dissemination activities, and exchange of good practices. This collaboration has started to be extended to the newly established CoEs, such as MultiXscale. 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. This recently happened e.g. in the participation in the ISC 23 common booth, and in the EuroHPC User Day on December 11, 2023 in Brussels (invited talk by Ivan Carnimeo - SISSA, and session chaired by Elisa Molinari).

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Fig. 1. MAX representatives @ ISC 23 (left) and EuroHPC User Day (right).

#### 4.1 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, Hackatons and Training Initiatives with National Competence Centres:** MAX provides domain-specific content and expertise on software development

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for exascale systems and beyond. MAX is contributing to the training activities coordinated with National Competence Centres.

- **Contribution to Courses, Hackatons and Training Initiatives with HPC Centres, and other CoEs:** MAX actively participates in training initiatives organised by HPC centres, the EuroHPC JU training platform and other CoEs. This collaboration ensures the integration of MAX domain-specific knowledge and expertise into broader training programs.
- **Contribution to Training Portals:** MAX contributes 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.
- **Training through Research:** MAX labs will offer research-oriented training to new developers interested in specific implementations within flagship codes, using contacts within user communities and through NCCs, CASTIEL 2 activities and EUMaster4HPC - related contacts. An established form within the MAX community is organising specialised schools in the field of materials science, with a specific focus on the new capabilities offered by (pre-) and exascale electronic structure codes. These events will typically include introductory sessions covering concepts and methods, as well as hands-on code-specific or code-group-specific training for both new and experienced users.

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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. To maximise engagement from user communities and increase the number of trained scientists and engineers, we plan to collaborate with established organisations in this domain, such as CECAM, Psi-k, and ICTP, and to support, continue and expand existing effort of the code developing and using communities, such as hackathons and summer schools..

Our CI/CD team, through CASTIEL 2, compared approaches of the other CoEs to exchange expertise and information. The CI/CD team attended two workshops organised by MultiXscale, and included the technical expertise in our testing framework and recommendations:

- Best Practices for CernVM-FS in HPC<sup>4</sup>
- Streaming Optimised Scientific Software: an Introduction to EESSI

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<sup>5</sup> 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 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<sup>6</sup>.

Furthermore **Laura Bellentani (CINECA)** and **Nicola Spallanzani (Cnr)** attended the course “**Introduction to Leonardo HPC cluster, for users and developers**” as tutors of the session “Overview of applications performance on Leonardo”. The course intended to support the scientific community to efficiently exploit the Leonardo supercomputer system. providing a full description of the system, with special emphasis on the main crucial aspects for users and application developers such as the access to the cluster, the architecture, and data resources, together with an overview of the software modules and of the programming and production environment. Bologna (IT), October 27, 2023.

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<sup>4</sup> <https://multixscale.github.io/cvmfs-tutorial-hpc-best-practices>

<sup>5</sup> <https://enccs.se/news/2022/12/efficient-materials-modelling-workshop/>

<sup>6</sup> <https://eurocc-netherlands.nl/calendar/mpi-and-openmp-in-scientific-software-development>



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Finally the **QuantumESPRESSO team** (Laura Bellentani - CINECA, Ivan Carnimeo and Oscar Baseggio - SISSA, Fabrizio Ferrari Ruffino - Cnr) attended the **LUMI GPU / Nomad CoE hackathon** held on September 4 - 6, 2023 at CSC, Finland.

Some more details are included in the report of the related WP7 activities, deliverable D7.3.

#### 4.2 Direct Involvement in NCC Activities

We plan to participate in larger national NCC events, joint NCC events and events where user communities within EuroHPC are involved (EuroHPC Days, EuroHPC User Forum) in order to present our activities, improve our visibility and demonstrate our solutions to the users as well as initiate contacts with academic and industrial communities.

MAX CoE has been presented or involved in the following NCC events:

- Arnes Network of Knowledge, November 14-16, Ljubljana, Slovenia (MAX presentation at the 3-day event on Open Science, Academic networks and Supercomputing, participation in use-case showcase, interaction with Multixscale CoE);
- Austria-Slovenia HPC days, 13-15 June 2023 at IZUM, Maribor, Sloveni (Presentation on MAX CI/CD and scalability efforts).

We plan to continue with this schedule, presenting MAX efforts, new code versions and scalability reports on national NCC events, inter-NCC events and conferences, as well as 2024 EuroHPC Days and EuroHPC User Forum.

We intend to contact CECAM to organise a joint activity with interested NCCs.

#### 4.3 Fostering Industrial Interaction

MAX as a High Performance Computing CoE funded by HORIZON-EUROHPC-JU-2021-COE-01 does not include industrial uptake as one of its core tasks. Nonetheless, we consider industrial uptake of our code and algorithms as an important way to increase and extend engagements with established and potential industrial end-users in our area as well as in the context of the European HPC infrastructure. 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. In the first year of the project, we have relied on our contacts with NCCs to provide the information in their communication with SMEs and industrial users.

Additionally, hardware (HW) manufacturers and software (SW) vendors are important actors in our area, both in the co-design activities and in the potential for economic impact of MAX

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applications if incorporated into commercial services and products. Interaction with relevant HW manufacturers has been ensured with their inclusion in the MAX consortium, and the existing and well established links with external industrial entities (e.g., NVIDIA, IBM) have been used through consortium members and hosting entities. We plan to expand these links and include the vendors and the companies that are potential users or disseminators of our codes in training and promotional activities wherever possible.

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 have implemented our intention 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.

#### 4.4 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<sup>7</sup>, a Twitter account<sup>8</sup>, a LinkedIn page<sup>9</sup>, and a YouTube channel<sup>10</sup>. 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.

Examples of the already established collaboration and support activities are:

- MAX visibility and coordinated attendance to the Euro HPC Summit Week 2023 - EuroHPC Joint Undertaking booth: poster with information about the CoE and brand identity;
- MAX visibility and coordinated attendance to ISC2023 - EuroHPC Joint Undertaking booth: video presenting MAX and brand identity.

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<sup>7</sup> [www.max-centre.eu](http://www.max-centre.eu)

<sup>8</sup> [https://twitter.com/max\\_center2](https://twitter.com/max_center2)

<sup>9</sup> <https://www.linkedin.com/company/max-centre>

<sup>10</sup> <https://www.youtube.com/channel/UCcoGe0aUy4gDVRNgjQIVf3g>

Deliverable D7.4: Update of collaboration plan (month 12)

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).

In order to participate in and extend such activities, we take the opportunity to present our work and events and conferences organised by or with the NCCs or HEs, such as the Austria-Slovenia HPC days.

## 5. Outlook & Next Steps

The collaboration of MAX with the CSA and other CoEs/NCCs set in the Grant Agreement has been progressing in the first 6 months and has evolved to regular and functional collaboration within the first year of the project. MAX continues 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. Some issues remain unresolved, but all relate to real technical challenges, namely in the CI/CD, central repository, access modes, HE technical coordination and software deployment methodology and support. We hope to bring these challenges to the front in order to resolve them to the advantage of all the CoEs and HEs.

Next steps:

- **Collaboration agreement (COLA):** due at M6 as from the specific milestone M7, it is undergoing review under the responsibility of the CSA and is expected to be available soon. WP7 leader L. Neri has followed the draft of the COLA on MAX side, continuously interacting with CASTIEL 2 relevant offices as a contact point between the CSA and the CoE's partners; revising it with Cnr Grant Support Office (dr. Giusy Lo Grasso); sharing it among partners and following deadlines and requests for finalisation. To date the final COLA has not been signed yet, but MAX coordinator is ready and supported with relevant Power of Attorney documents by its partners.

RP1 WP7 MILESTONE STATUS					
Milestone n.	Milestone Title	Lead Beneficiary	Due Date	Status	Actual delivery

Deliverable D7.4: Update of collaboration plan (month 12)

					date
MS7	Collaboration agreement has been signed.	CNR	M6	Approaching finalisation	M12

Fig 2. Milestone 7 definition from the MAX DoA.

- **Definition of common KPIs.** Targets for collaboration-related KPIs (K3.1, K3.2, K3.3, K3.4) have been defined. They are due within month 12 according to MAX DoA and have been coordinated with the CSA.
- **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	done
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.