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GA n. 101093374S



EuroHPC
Joint Undertaking

Deliverable D7.6: Second update of collaboration plan
(M30)

D7.6

Second update of collaboration plan (M30).

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List of abbreviations

AHM - All hands meeting
BSC – Barcelona Supercomputing Center
CAB – Competence Centres and CoE Advisory Board
CASTIEL 2 - Coordinating Action for Scientific and Technological Innovation for Exascale and Leading Technologies
CECAM – Centre Européen de Calcul Atomique et Moléculaire
CI/CD - Continuous Integration/Continuous Deployment
CNR – Consiglio Nazionale delle Ricerche (National Research Council of Italy)
CoE - Centre of Excellence
COLA – Collaboration Agreement
CPU - Central Processing Unit
CSA - Coordination and Support Action
CVMFS – CernVM File System
DFT - Density Functional Theory
DoA – Description of Action
DPU – Data Processing Unit
EESSI - European Environment for Scientific Software Installation
EU – European Union
EUPEX – European Exascale Pilot
EUPILOT – European Pilot Project for Exascale
EuroCC – European National Competence Centers
EuroHPC JU - European HPC Joint Undertaking
FPGA – Field-Programmable Gate Array
GA - Grant Agreement
GDPR - General Data Protection Regulation
GPU - Graphics Processing Unit
HE – Hosting Entity
HiPEAC – High Performance and Embedded Architecture and Compilation
HLRS - High Performance Computing Center Stuttgart



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HPC - High Performance Computing

HW – Hardware

ICTP - The Abdus Salam International Centre for Theoretical Physics

IP - Intellectual Property

ISC – International Supercomputing Conference

JUBE – Jülich Benchmarking Environment

KPI - Key Performance Indicator

MFA – Multi-Factor Authentication

NCC – National Competence Centre

NVDIMM – Non-Volatile Dual Inline Memory Module

PRACE - Partnership for Advanced Computing in Europe

PWTK – Pseudo Wavefunction Toolkit

R&D - Research and Development

RISC-V – Reduced Instruction Set Computing (open-source processor architecture)

SISSA – Scuola Internazionale Superiore di Studi Avanzati (International School for Advanced Studies)

SLURM – Simple Linux Utility for Resource Management

SME – Small and Medium Enterprises

SPACE – Simulation for Particle Accelerators and Computing Engineering

SSH – Secure Shell

SW – Software

WG - Working Group

WP - Work Package



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1. 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 mechanical simulation) codes (QUANTUM ESPRESSO, Yambo, Siesta, Fleur, BigDFT) 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 collaborates with the complementary projects and the dedicated Coordination and Support Action (CSA) CASTIEL 2 (Grant No. 101102047) by developing the following activities:

- Contributing to CASTIEL 2 coordination activities as CSA and the C2ISS¹ portal.
- Participating in regular meetings to plan, implement and monitor collaborations, and to synchronise research and development activities addressing cross-cutting issues.
- Participating in benchmarking exercises, sharing results and best practices.
- Participation in joint events, publication and dissemination activities.
- Continuous integration and application deployment platform for Lighthouse codes on EuroHPC JU systems.
- Establishing best practices for IP management and development, including effective measures to ensure code quality, reviews, testing, management and development cycles.
- Code modularisation: identification of common routines, algorithms and modules, and creation and extension of software libraries used by multiple codes across disciplines.

This deliverable outlines the implementation of these activities by month 30 and the plans for the remainder of the project.

¹ <https://hpc-portal.eu/>



2. 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. One of its main goals is to collaborate with other complementary CoEs and with 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:

- Active contribution to the coordination activities of CASTIEL 2 as CSA
- Contribution to the common C2ISS portal
- Establishment of effective collaborations and jointly addressing cross-cutting issues with CSA and its coordinated actions
- 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 on all EuroHPC JU systems.
- 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 safeguard 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:



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1. The CSA's and CoE's Grant Agreements, which describe mechanisms and goals for collaboration.
2. The Collaboration Agreement – due at M6 and signed at M20 – 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) were added to the MaX list of KPIs (see Section 4.4):

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 the 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 KPI format has been adopted by CASTIEL 2 to monitor their progress, and we have started to report on the status for CASTIEL 2 to be able to gather the status from all contributing CoEs.

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

3. 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 in by all our Work Packages (WP) to be actively and fruitfully involved and to communicate the joint activities to all the partners and coordinate the project evolution. The action requires actively contributing to the coordination activities of the associated CSA. CASTIEL-



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

MaX played a key role in the activities of FocusCoE (2018-2022), benefiting from the development of common actions, interactions with other CoEs, support in sustainability, communication, training, and other activities. In this framework, we actively and consistently collaborate with CASTIEL 2 in structuring the common HPC ecosystem and boosting the 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 (updated to June 2025).

CASTIEL2 WP	MaX appointed Champion	MaX appointed deputy
WP2 "NCCs/CoEs 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 and Outreach"	Marina Corradini (ICN2) NEW	Luisa Neri (CNR)

Fig. 1. MaX "Champions" and deputies in CASTIEL2 WPs.

We have since attended all CASTIEL2 meetings:

- Kick-off in Stuttgart, Germany, 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.

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- Communication workshop CoEs, NCCs and CASTIEL2 in Brussels, March 22, 2024. Luisa Neri (CNR) and Marina Corradini (ICN2) discussed communication-related topics, planned for collaborative activities, and learned more about tools such as Canva & WordPress.
- CoE technical collaboration: First meeting on GPU programming, July 4, 2024, online. Nicola Spallanzani (CNR) and others attended the meeting as representatives of MaX.
- CASTIEL2, EuroCC2 and CoE, All Hands Meeting (AHM) in the Tatra mountains in Slovakia, April 22-24, 2024. Luisa Neri (CNR) attended in person to introduce MaX and evaluate collaborations with NCCs and CoEs.
- EuroCC Italy and CoEs, May 8, 2024, online. Andrea Ferretti (CNR) and Nicola Spallanzani (CNR) presented MaX CoE to the Italian NCC and other CoEs (ChESEE, EoCoE, EXCELLERAT, and SPACE) to explore potential collaborations.
- 2nd NCCs-CoEs meeting, November 8, 2024, online. Nicola Spallanzani and Luisa Neri (CNR) and Marina Corradini (ICN2) attended a meeting where new CoEs (EoCoE, POP-III, MICROCARD-2 and dealii-X) were presented, as well as the European Support Centres EPICURE and MINERVA.
- Communication Champions Meeting, gathering the Communications Champions and Deputies from all CoEs, NCCs and CASTIEL2 in Barcelona, June 30, 2025. Luisa Neri (CNR) and Marina Corradini (ICN2) will represent MaX CoE.

Also, a list of attended regular meetings and activities performed in the framework of the 3 different CASTIEL 2 WPs is presented below:

- **Castiel 2 Project Management Team (PMT) - COE meetings:** monthly meetings (from now on, every first Tuesday of the month) in which common topics about the management of the network are discussed. Attended by Luisa Neri (CNR).
- **WP3 Training, Twinning Mentoring COFFEE BREAKS:** monthly meetings on the first Thursday of the month, starting from May 2023. Outstanding meetings in this series are highlighted in the following:
 - 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.



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- 30/11/2023 special meeting: Daniele Varsano (WP5 Leader) and Luisa Neri (WP7 Leader) with the new CASTIEL2 WP Leader Aline Melinette;
- **WP4 NCCs, COEs and industry interaction COFFEE BREAKS:** monthly meeting on the fourth Thursday of the month, starting from September 2023.
- **WP5 Awareness, impact, outreach & sustainability COFFEE BREAKS:** bimonthly meeting starting from May 2024. Outstanding meeting highlighted in the following:
 - 21/06/2024 special meeting with CASTIEL2 and all CoEs.

And further collaborations with CASTIEL 2:

- Barbara Krasovec (IJS) participated in the CASTIEL2 CI/CD working group (WG) for MaX. The main focus of the biweekly meetings (initiated in July 2024) was to establish a common CI/CD solution for all CoEs. While most CoEs have their solution in place, the WG decided to provide a common solution for delivery. The goal of the WG was also to provide best practices and examples of how to run CI. A documentation section is being prepared at <https://codehub.hlr.de/castiel2/documentation>. The Castiel2 CodeHub will also provide the European Environment for Scientific Software Installation (EESSI) and Jacamar runners for those CoEs that wish to use their GitLab instance for CI processes.
- Marina Corradini (ICN2) is part of the CASTIEL2 “[Supercomputing in Europe Podcast](#)²” task force. The podcast is a joint communication activity between CASTIEL2, the Centres of Excellence (CoEs), and the National Competence Centres (NCCs). The task force meets regularly to coordinate and support the podcast’s production. These meetings cover episode planning, potential speakers, and organisational updates behind the scenes.

² <https://open.spotify.com/show/4pZ7nfUZTs3tDyfWVfAR8q>



Fig. 2. Promotional banner on MaX episode of the CASTIEL 2-NCC-CoE podcast series "Supercomputing in Europe" (June 18, 2025).³

- Pablo Ordejón (ICN2) presented the MaX lighthouse code SIESTA in "SIESTA: a DFT code for large-scale computational material science in HPC environments", as part of the "CASTIEL2 Code of the Month" webinar series (11/12/2024).
- Marina Corradini (ICN2) organised for MaX, along with other CoEs, two workshops within the HiPEAC 2025 conference held in Barcelona. The

workshops From petascale to exascale and beyond: the Centres of Excellence challenge and Tackling software exascale challenges: the Centres of Excellence in High Performance Computing perspective spotted a wide panel of all-female scientists and experts, so tackling the gender in HPC issue along with high-level scientific topics (21-22/01/2025).

- Luisa Neri (CNR) has been elected as CoE deputy member of the CAB "Competence Centres and CoE Advisory Board" (CAB). The CAB has the role to discuss and monitor the progress, achievements and plans of CASTIEL 2, by meeting at least every 3 months with the CASTIEL 2 leaders (the C5 body). It is composed of 4 elected representatives from all the NCCs and 4 elected representatives from the CoEs. The CAB has so far met 6 times.

We will continue attending CASTIEL2 meetings, participating in thematic meetings, collaborating with NCCs and other CoEs, and continuing to contribute feedback to all requests.

³ https://open.spotify.com/episode/OwdKpNooCibrjoT5qHeAvj?si=_0gNBfI4RDuN0LtIYOfMAQ

4. Technical deployment

4.1 Advanced Technologies Monitoring

MaX has a strong focus on identifying interesting technologies that have the potential to become mainstream in the next few years and can be currently used as co-design platforms, advanced hardware platforms, and systems suitable for energy-efficiency evaluation. All these goals are tackled in WP4. Within this effort, we engage in contacts with HPC sites, universities, technology partners, vendors, and integrators to gain access to these cutting-edge platforms. These platforms are primarily utilised for benchmarking purposes via mini-apps extracted from MaX codes. For brand new platforms, but with a more robust software ecosystem, entire applications are ported and used to validate these software stacks as well as individual features of novel HW architectures.

Several interesting architectures and novel technologies are provided to the effort by consortium partners (i.e., A64FX CPUs, Intel's 512GB NVDIMM persistent memory modules, Bittware 520N-MX FPGA cards, FPGA Xilinx Alveo U250 Data Center Accelerator Cards, NVIDIA BlueField-2 DPU, Power 10 CPUs, ARM Neoverse-N1 80-Core CPUs, AMD MI200 GPUs). This original set has been extended by the new GPU-accelerated (NVIDIA Grace-Grace or GraceHopper, AMD MI300A or MI300X, etc.) and new CPU platforms, out of which we must mention RISC-V based CPUs, as this is becoming an essential architecture for European countries with EUPILLOT and with the recent start of the EuroHPC DARE project [more details in *D1.3 Second report on software architecture and implementation planning* (M30) and *D4.3 First Co-design report* (M30)].

In cases when access cannot be directly provided by MaX partners, collaboration with outside entities and industrial actors is always explored. In some instances (E4), direct access can be provided, in others (EVIDEN), case-by-case solutions have been arranged within MaX. We are in close contact with the European pilot for the exascale (EUPEX⁴) project and gained access to the EUPEX software development vehicles to evaluate its software stack. Similarly, we expect to coordinate with SiPearl to have their personnel perform runs on their development boards when the Rhea chip becomes available.

We continuously search for new interesting platforms at a small scale, but also investigate large systems with new HW architectures to support WP1 in porting to next-generation HPC systems

⁴ <https://eupex.eu/>

by reducing their porting time. In all cases, we seek further collaboration with vendors, HPC centres, and developers to gain early access to new technologies for this effort.

4.2 CI/CD Platform

Continuous Integration and Continuous Deployment (CI/CD) practices have become increasingly relevant in HPC, where code integrity, performance optimisation, and efficient deployment are crucial. 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 essential 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 so the code can be compiled with minimal intervention.

For the benchmarking effort within MaX, we adopted JUBE⁵, a tool developed at the Jülich Supercomputing Centre 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 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 is available in the *JUBE4MaX*⁶ repository, dedicated to MaX JUBE material, and can serve as an example for setting up HPC benchmarking for advanced codes on multiple architectures.

To facilitate the deployment of CoE codes on all the EuroHPC supercomputers, CASTIEL 2 started driving the implementation of a unified CI/CD platform. Since many HPC centres are already providing a CI/CD procedure for their users, CASTIEL 2 decided to pair the HPC centres with one

⁵<https://www.fz-juelich.de/en/ias/jsc/services/user-support/software-tools/jube?expand=translations,fzjsettings,nearest-institut>

⁶https://gitlab.com/max-centre/JUBE4MaX/-/tree/develop?ref_type=heads



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or more CoEs to start some tests. Based on these preliminary tests, CASTIEL 2 collected all the data to develop the platform in collaboration with all the stakeholders. Pairing a CoE with a EuroHPC hosting site should allow both parties to learn from each other. On the one hand, the CoE will get hands-on experience with the existing CI/CD environment. On the other hand, the HPC site gets insights into specific requirements imposed by codes from the CoE. For this, all involved persons explored the corresponding CI/CD for 4-5 weeks, and after that, CASTIEL 2 requested reports on their experience. CASTIEL 2 paired the MAX and ESIWACE CoEs with the CINECA supercomputing centre to start this collaboration. After the establishment of the CI/CD working group, it was decided to focus on the CD and leave freedom to the developers on the use of their own CI, or to use the proposed CASTIEL 2 Codehub for the same purpose. The outcomes from the work carried out by these working groups are currently being compiled, and the documentation is being put together in a shared portal, which will become publicly available soon.

This task aims to effectively deploy and tune the MaX Lighthouse codes and workflows on EuroHPC systems. This work includes supporting the execution of workflows inspired by scientific grand challenges and their optimisation. We envisage the production of environment modules and container-based solutions for HPC deployment of MaX applications. To support this effort, our members participate in the EuroHPC HPC Container Forum (regular monthly meetings, including a face-to-face meeting at the EuroHPC Summit 2025). In addition, we have been working on incorporating security controls into the CI/CD process – the CI jobs are executed in a Docker container, and the container image is scanned for vulnerabilities and secrets. We also started to set up the underlying infrastructure by providing a vault to store secrets and implementing OS hardening, MFA, access control, and security policies on the local GitLab instances and machines used for runners.

In our exchanges with CASTIEL 2 and the other CoEs, we contacted MultiXscale⁷ CoE, which promotes the CernVM File System (CVMFS) distributed storage 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, which will also be supported by the EuroHPC Federation Platform. 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

⁷ <https://www.multixscale.eu/>

centralised/orchestrated software deployment and would profit from the fact that CVMFS is suitable also for small files. This makes the use of sandboxed software containers using CVMFS easy, straightforward, and efficient. The solution is already supported on the Vega and Karolina sites. This task will also contribute to the execution of benchmarks, reporting the results in terms of performance efficiency as well as power efficiency, on the EuroHPC systems.

Internally, 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 the 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.

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.

4.3 Special Access Scheme

Following our attempt to obtain preferential access to the machines through CASTIEL 2, we were informed that this type of access was not intended for CoEs. We therefore secured the necessary access through the EuroHPC calls for Development and Benchmarking. Obtaining these resources allowed the MaX codes to be ported and deployed on different architectures, addressing possible issues and working towards their resolution. As part of the MaX T3.4 deployment on EuroHPC machines, we have requested access to EuroHPC machines by applying to the development access calls, adding 8 different partitions to the existing 6 (on a total of 7 EuroHPC machines), to build our codes and run the corresponding benchmarks. The Leonardo⁸ supercomputer at

⁸ <https://www.hpc.cineca.it/systems/hardware/leonardo>



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CINECA was initially proposed as the initial system for the profiling and benchmarking activities within MaX WP3. Leonardo had the largest HPC architecture available at the early stages of MaX, and direct access was given to all MaX code and CI/CD developers. In addition, the EuroHPC systems Vega, hosted at IZUM/SLING, and Karolina, hosted at IT4Innovations, provided direct access to other MaX partners to test their machines. In addition, intensive work on the MareNostrum5⁹ supercomputer at BSC was also carried out in line with the deployment and benchmarking activities of *WP3 Technical challenges towards exascale and postexascale*. In this case, tasks were initiated by the BSC partners that could take advantage of the early access to the resources in the pre-benchmark phase, and this was taken over in cooperation with the code developers when EuroHPC access became available. Also, the peta-scale EuroHPC systems Vega, hosted at IZUM/SLING, and Karolina, hosted at IT4Innovations, provided direct access to other MaX partners to test their machines.

4.4 Definition of common KPIs

Common KPIs have been defined, including the targets for the collaboration-related KPIs (K3.1, K3.2, K3.3, K3.4), in line with the timeline set in the MaX DoA (due by month 12). Their definition has been successfully completed and coordinated with the CSA.

KPI n.	Description	Target M12	Value M12
K3.1	No of applications deployed to JU systems incl. breakdown by partition (e.g. CPU, GPU).	intermediate targets: 5 codes * Target % coverage * Number of available partitions	1.73 Modules, 2.36 Demonstr, 4.45 Supported
K3.2	No of EUROHPC systems supported by application incl. breakdown by partition (e.g. CPU, GPU).	Intermediate targets: No of available EuroHPC partitions * Target % coverage	3.8 Modules, 5.2 Demonstr, 9.8 Supported
K3.3	No of errors (failed deployments/ regression tests) identified through common platform.	intermediate targets are all equal to Target M48	N.A.
K3.4	Average time from failed application test to deployment of corrected application.	intermediate targets are all equal to Target M48	N.A.

⁹ <https://www.bsc.es/supportkc/docs/MareNostrum5/overview/>



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K3.0	Average % coverage of EuroHPC systems	40%	11 partitions, 35% Modules, 47% Demonstr, 89% Supported
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KPI n.	Value M18	Value M24	Target M48
K3.1	1.77 Modules, 3.08 Demonstr, 4.69 Supported	1.81 Modules, 3.19 Demonstr, 4.75 Supported	All MAX codes will be deployed to JU systems, on both cpus and gpus partitions. TARGET = 5.0
K3.2	4.6 Modules, 8.0 Demonstr, 12.2 Supported	5.8 Modules, 10.2 Demonstr, 15.2 Supported	All MAX codes will be deployed to JU systems, on both cpus and gpus partitions. TARGET = # partitions
K3.3	N.A.	N.A.	5-10 bugs/year (1-2 bugs per code per year)
K3.4	N.A.	N.A.	2 months
K3.0	13 partitions, 35% Modules, 62% Demonstr, 94% Supported	16 partitions, 36% Modules, 64% Demonstr, 95% Supported	100%

Table 2. List of common KPIs descriptions, targets and intermediate values that show the evolution towards achieving the targets.

5. 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, 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 HPC CoE Council (HPC3) since its foundation, and will continue to do so, providing advice and contributing when relevant. The same effort will be made in participating in actions promoted and organised by the EuroHPC JU. This recently happened, e.g., in the



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participation in common booths at the ISC23 and ISC24¹⁰ conferences, and in the EuroHPC User Days.

The first was held in Brussels (11/12/2025) to bring together the EuroHPC user community to showcase the projects using European supercomputing resources and featured an invited talk by Ivan Carnimeo (SISSA) and a session chaired by Elisa Molinari (CNR & UNIMORE). The second took place in Amsterdam (22-23/10/2024). Together with other CoEs, MaX hosted a special session for users called “Walk-in networking sessions focusing on specific EuroHPC user needs: provide your feedback and get some advice.” The special session featured again the interventions of Molinari and Carnimeo as representatives of MaX. They presented the latest results of the MaX lighthouse codes in achieving performance and scaling on different EuroHPC architectures.

MaX partners also collaborate actively with the PoP¹¹ CoE, ensuring that sophisticated materials science applications are effectively optimised to harness the full potential of exascale architectures. One prominent example of their collaboration is their joint participation in the HiPEAC 2025 Conference, alongside other CoEs such as ChEES¹², ESiWACE¹³, MultiXscale, EXCELLERAT¹⁴, EoCoE¹⁵, POP3, and SPACE¹⁶. During the conference, the CoEs organised two special workshops to give voice to women experts in High-Performance Computing (HPC) and discuss the challenges and the initiative proposed by the European CoEs addressed ongoing gender disparities in HPC, where women remain underrepresented, particularly as keynote speakers at conferences. By normalising women’s voices in the field, the CoEs aim to inspire and empower the next generation of women in STEM. In addition, previous collaboration with other CoEs on computational materials science, such as the NOMAD CoE, facilitated the implementation of libraries such as ELPA on MAX flagship codes.

¹⁰ <https://isc-hpc.com/>

¹¹ <https://pop-coe.eu/>

¹² <https://www.cheese-coe.eu/>

¹³ <https://www.esiwace.eu/>

¹⁴ <https://www.excellerat.eu/>

¹⁵ <https://www.eocoe.eu/>

¹⁶ <https://www.space-coe.eu/>

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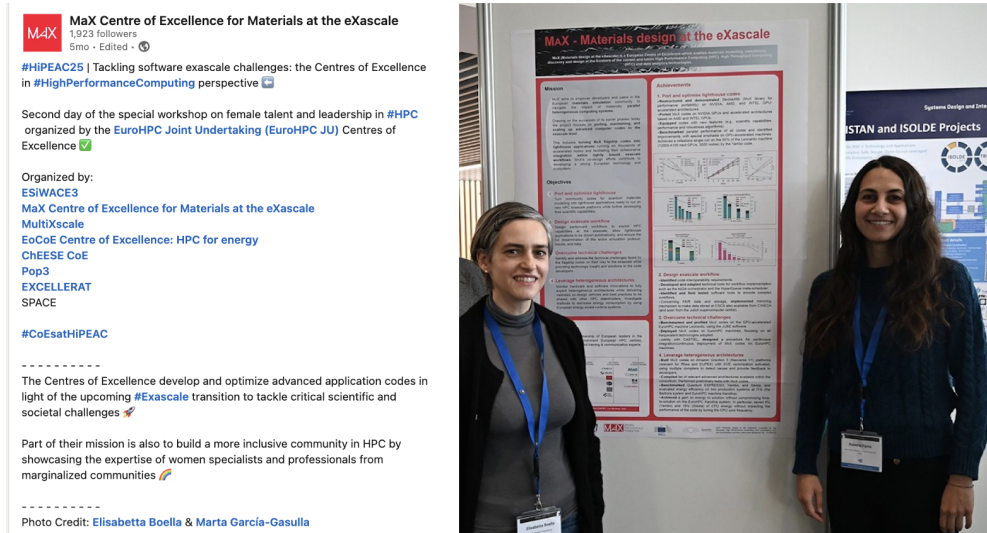


Fig. 3. MaX (and joint CoEs) post for HiPEAC 2025 workshops (left) and Farris (ICN2) and Boella (E4) at HiPEAC 2025 (right).

5.1 Enabling Exchange of Expertise

One of the main features of MaX is to provide training for users, developers, researchers, and students for its lighthouse codes. MaX has a well-grounded tradition in this field, developed by exploiting in a systematic and coordinated way the training actions organised by its partners. Schools, hackathons, research lab experiences, and participation as tutors and mentors to third-party events are coordinated by *WP5 Training & Community engagement* within the HPC ecosystem, led by Daniele Varsano (CNR). T5.3 is devoted to 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 NCCs, HPC centres, other CoEs, EuroHPC Training Activities and Professional Traineeships funded by the Digital Europe Programme.

Our focus is on domain-specific content, software development know-how for exascale systems, and integration of new knowledge into universities and higher education. The following activities in these lines are being undertaken:



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- **Contribution to courses, hackathons and training initiatives with NCCs, HPC centres, and other CoEs:** MaX provides domain-specific content and expertise on software development for exascale systems and beyond. MaX actively participates in training initiatives organised by HPC centres, the EuroHPC JU training platform and other CoEs, and contributes to the training activities coordinated with NCCs. These collaborations ensure the integration of MaX domain-specific knowledge and expertise into broader training programs.
- **Contribution to Training Portals:** MaX contributes to the training portals of NCCs' and CoE's community¹⁷ 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, e.g., Virtual Training coffee breaks.
- **Development of flexible teaching modules:** MaX recognises the importance of integrating new knowledge into universities and higher education. Flexible teaching modules based on MaX lighthouse codes will be developed and tested. These modules will target MSc. /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 MSc. or Ph.D. courses based on HPC will be fostered, and collaborations with the European Master for HPC ([EUMaster4HPC](https://eumaster4hpc.uni.lu)¹⁸) 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 materials science, with a specific focus on the new capabilities offered by (pre-)exascale electronic structure codes. These events will typically include introductory

¹⁷ <https://hpc-portal.eu/training>

¹⁸ <https://eumaster4hpc.uni.lu>

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sessions covering concepts and methods, as well as hands-on code-specific or code-group-specific training for beginners and experienced users.

The outputs of this task will include contributions to training initiatives coordinated with NCCs and the wider European HPC ecosystem. 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.

Key Actions Undertaken:

- Uploaded all MaX training events to the HPC Training Portal.
- Actively participated in CASTIEL2 “Training Coffee Break” meetings held monthly since May 4, 2023.
- Presented “MaX Training: Plan and Strategies” at the CASTIEL2 “Training Coffee Break” on October 5, 2023 [D. Varsano, CNR].

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, which included the technical expertise in our testing framework and recommendations:

- Best practices for CVMFS in HPC¹⁹
- Streaming optimised scientific software: an Introduction to EESSI

Fruitful collaborations were established with NCCs. MaX contributed to the EuroCC & CASTIEL2 "Training Sprint Initiative" with three events and coordinated with NCCs for 3 training events focused on MaX's flagship codes. All the training material is available online in the Lhumos platform²⁰.

- MaX school: Materials and molecular modelling with QUANTUM ESPRESSO²¹. Online, 18-21/06/2024. In collaboration with NCC Austria, NCC Czechia, NCC Hungary, NCC Poland, NCC Slovakia, and NCC Slovenia. Participants: 46.

¹⁹ <https://multixscale.github.io/cvmfs-tutorial-hpc-best-practices>

²⁰ <https://lhumos.org/>

²¹ <https://events.it4i.cz/event/252/>



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- MaX/HPC-NCC-Croatia QE workshop (Modelling of (nano)materials with Quantum ESPRESSO).²² Zagreb (Croatia), 12-13/11/2024. Participants: 8.
- SIESTA School 2024.²³ Online, 11-15/11/2024. In collaboration with NCC Spain. Participants: 151.

MaX also coordinated with NCCs for three additional training events focused on MaX flagship codes

- Efficient materials modelling on HPC with QUANTUM ESPRESSO, SIESTA and Yambo.²⁴ Online, 11-15/03/2024. In collaboration with NCC Sweden. Participants: 78.
- Machine Learning Modalities for Material Science²⁵. Ljubljana (Slovenia), 13-17/05/2024. In collaboration with NCC Slovenia. Participants: 132.
- PWTK-2024: An Online Tutorial²⁶. Online, 20-24/05/2024. In collaboration with NCC Slovenia. Participants: 95.

Furthermore, in 2023 and 2024, 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 into details about algorithmic design and implementations²⁷.

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 is intended to support the scientific community in efficiently exploiting 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 access to the cluster, the architecture, and data resources, together with an overview of the software modules and the programming and production environment. The course took place in Bologna, Italy, on October 27, 2023. Finally, the Quantum ESPRESSO team (Laura Bellentani - CINECA, Ivan Carnimeo and Oscar Baseggio - SISSA, Fabrizio Ferrari Ruffino - CNR) attended the LUMI GPU / Nomad CoE hackathon held at CSC, Finland, 4-

²² https://www.hpc-cc.hr/NCC_Croatia_HPC_day_2024

²³ https://siesta-project.org/siesta/events/SIESTA_School-2024/

²⁴ <https://encs.se/events/2024-03-efficient-materials-modelling-on-hpc/>

²⁵ <https://ml4ms.ijs.si/>

²⁶ <http://pwtk.ijs.si/pwtk-2024.html>

²⁷ <https://eurocc-netherlands.nl/calendar/mpi-and-openmp-in-scientific-software-development>



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6/9/2025. More details on these are included in the deliverable *D7.3 Report on the setup of MaX CoE*, devoted to WP7 activities.

5.2 Direct Involvement in NCC Activities

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

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

- Arnes Network of Knowledge, November 14-16, 2023, 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, Slovenia (Presentation on MaX CI/CD and scalability efforts).
- Castiel 2 code of the month: Siesta 11/12/2024. The MaX Centre and the Siesta code were presented in the webinar series organised by CASTIEL 2.

MaX work and achievements have also been presented in the following events organised by the EuroHPC JU and related ecosystem:

- Euro HPC Summit Week 2023, 20-23/03/2023, Göteborg (SE).
- Euro HPC User Day, 11/12/2023, Brussels (BE).
- Euro HPC Summit Week 2024, 18-21/03/2024, Antwerp (BE).
- Second EuroHPC User Day, 22-23/10/2024, Amsterdam (NL).
- EuroHPC Summit Week, 18-20/03/2025, Kraków (PL).

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Fig. 4. MaX group at EuroHPC 2025.

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 in the upcoming EuroHPC Days and EuroHPC User Forum. We also intend to contact CECAM to organise a joint activity with interested NCCs.

5.3 Fostering Industrial Interaction

While MaX does not include industrial uptake as one of its core tasks, we consider this an important way to increase and extend engagements with established and potential industrial end-users in our area, and 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 the exploitation of MaX results. In the M30 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 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 keep expanding these links and

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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, focus on companies within the European Union and the Participating States of the EuroHPC Joint Undertaking. Therefore, we have so far actively attended and contributed to most of the activities promoted by CASTIEL 2 in its WP4 NCCs, COEs and industry interaction, from surveys to webinars, sectoral events, and more.

5. 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 website²⁸, a X account²⁹, a LinkedIn page³⁰, a YouTube channel³¹, and since January 2025, a BlueSky account³². MaX achievements and updates are also disseminated through the MaX LinkedIn Newsletter³³. These activities are led by *WP6 Communication, exploitation, and dissemination*, coordinated by Marina Corradini (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 in 2023, 2024, and 2025, where MaX was featured together with its fellow CoEs at the EuroHPC JU booth.
- MaX visibility and coordinated attendance to ISC2023, ISC2024, and ISC2025: through the booths of the EuroHPC JU and partner IT4Innovation, where MaX was showcased through a video and brand material.
- Together with its fellow CoEs ESIWACE, EXCELLERAT, EoCoE, MultiXscale, POP3, and SPACE, MaX organised two special workshops at the HiPEAC2025 to promote women's expertise and leadership in HPC. The workshops were dedicated to highlighting the latest

²⁸ www.max-centre.eu

²⁹ https://twitter.com/max_center2

³⁰ <https://www.linkedin.com/company/max-centre>

³¹ <https://www.youtube.com/channel/UCcoGe0aUy4gDVRNgiQIVf3g>

³² [MaX - Materials design at the eXascale \(@max-coe.bsky.social\) — Bluesky](#)

³³ <https://www.linkedin.com/build-relation/newsletter-follow?entityUrn=7221808079808393219>

advances in HPC while praising the contributions of women scientists and engineers in the field.

- As part of the joint communication initiative “Supercomputing in Europe” podcast, Marina Corradini (ICN2) and Roberta Farris (ICN2) contributed with the production of one podcast episode, “Supercomputing for Materials Design”, released on June 18, 2025 and available on [EuroCC & CoEs Spotify](#)³⁴ and the various EuroCC and MaX digital channels.

Interaction with supercomputers and NCCs is crucial for MaX, as they are key actors in the dissemination of our scientific and software production, our engagement with our community of users, and the participants in our training events, schools and hackathons. NCCs are 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 have been 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). To participate in and extend such activities, we took the opportunity to present our work and events and conferences organised by or with the NCCs or Hosting Entities (HEs), such as the Austria-Slovenia HPC days. In addition, MaX regularly contributes to CASTIEL2’s social media channels (LinkedIn³⁵ and BlueSky³⁶), the joint “NCCs & CoEs Newsletter”. These efforts help to increase the visibility of MaX results and support the digital growth of CASTIEL2.

6 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 up to now. MaX continues to play its role both in the technical deployment and in the training, exploitation, and 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 to resolve them to the advantage of all the CoEs and HEs.

³⁴

<https://open.spotify.com/show/4pZ7nfUZTs3tDyfWVFAR8q?si=cdafea7116734fc0&nd=1&dlsi=de17b48ffcc14b07>

³⁵ <https://www.linkedin.com/company/hpc-coe/posts/?feedView=all>

³⁶ <https://bsky.app/profile/hpccoe.bsky.social>



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The **Collaboration agreement (COLA)** was eventually signed in August 2024 by all institutions belonging to the CoEs and is now being adopted by new CoEs. It was drafted to enable the parties to comply with clauses in Article 7 and the Data Sheet (Point 1), included in all respective Grant Agreements. It outlines the framework for collaboration between CASTIEL 2 and the involved CoEs.

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	done
D7.9	Final report of collaboration plan	BSC	48	

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