D7.3

Report on the setup of the MAX CoE

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Content

1. Executive Summary

The deliverable D7.3 summarises the setting up of the MAX Centre of Excellence (CoE), established through the HORIZON-EUROHPC-JU-2021-COE-01 call for the four year period 2023-2026. The Centre was not created anew: it is actually based on two previous MAX CoE editions (H2020 2015-2018 and 2018-2022). We therefore move from that experience to address significant changes and new challenges that affect the CoE organisation. Among these, we point out the new consortium composition and the modified rules and objectives. Importantly, the CoE now lies within the EuroHPC Joint Undertaking and will therefore develop strong collaborations with its ecosystem and with the Castiel-2 CSA.

This third phase of MAX allows the management team and the whole consortium to take advantage of the experience acquired, analyse strengths and weaknesses of the previous project phases, and to consolidate the management structure while implementing *ad hoc* corrections to take into account the new call requirements and the new consortium composition.

In the deliverable we present the establishing of governing bodies; the internal organisation structure; activities performed within WP7 Management, including references to the initial collaboration with the Castiel2 CSA. A description of the KPIs as set by the consortium is also given and discussed.

2. MAX consortium

MAX - *Materials design at the exascale* Centre of Excellence, as established within the HORIZON-EUROHPC-JU-2021-COE-01 call, is coordinated by Cnr (IT), and consists of 14 partners and 2 affiliated entities (Unimore and CSIC), as depicted below. The partners consist of “domain experts and code developers” (Cnr, Sissa, ICN2, Juelich, CEA, UBremen), “HPC experts & data centres” (CINECA, Juelich, CEA, BSC, IT4I, JSI), “technology & co-design partners” (ATOS, Sipearl, E4, Leonardo). They are from six EU countries: Italy, France, Spain, Slovenia, Czech Republic, and Germany.

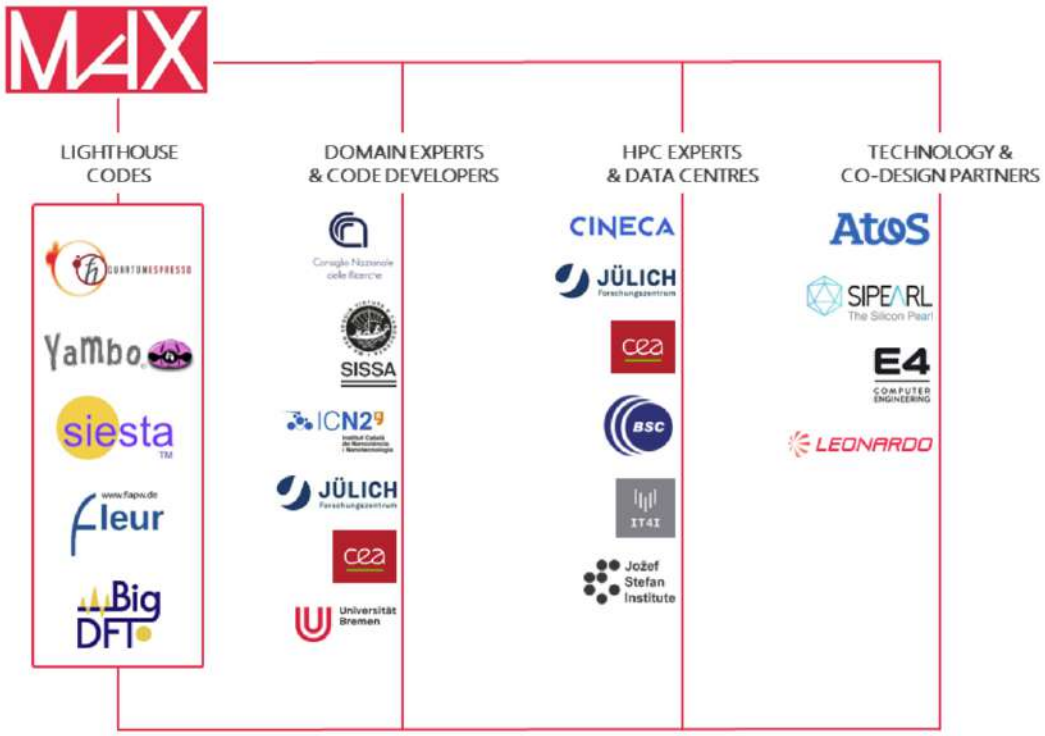


Fig. 1. Structure of the MAX Centre of Excellence.

Several of these partners have been part of MAX since its first (2015) or second edition (2018): MAX as a network can thus rely on a solid tradition as a CoE and its set-up has not been implemented from scratch. The CoE has evolved into the new configuration, adding new partners and improving its strategies and activities on the basis of the acquired experience.

To get an idea of the evolving consortium in years, the composition in different editions is pictured below. We point out that the code-developing teams have been part of MAX since the beginning. Some of the industrial team participation has evolved as a consequence of the European and EuroHPC membership and policies. Also, the participation of the Swiss teams (EPFL and ETHZ-CSCS) and ICTP was excluded according to the requirements of the call.

The PI, Elisa Molinari, and its team have consolidated in years, developing strong skills in management and internal communication. In the next chapters, a report of activities performed within the WP7, aimed at setting up and running the CoE as an institution, will be given task by task.

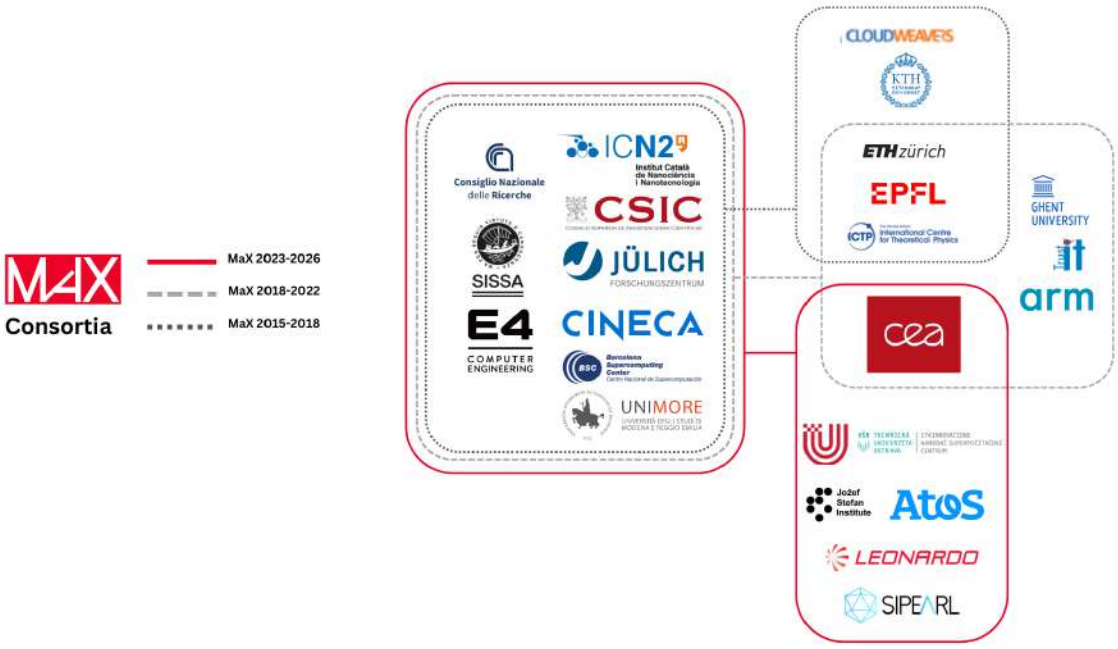


Fig. 2. Structure of the MAX Centre of Excellence in different editions.

3. CoE Governing Bodies

As defined in the DoA (section B.3.1, Work plan and resources and Description of the Work packages) and agreed upon by the partners in the Consortium Agreement (art. 6.1) the organisational structure of this Consortium is composed by:

1. the General Assembly (GA),
2. the Work-Package Leaders Committee (WP-Exec).
3. the Coordinator.

Three additional bodies/operational structures are set up informally by the Consortium to ease the project implementation and to flank the Coordinator:

4. the WP Committees,
5. the Technical Project Manager,
6. the Software Technical Board (STB),
7. the Management Team.

Below, we provide a description of each established body and of work performed in the first 12 months of activity:

1. The **General Assembly** (GA) is the ultimate decision-making body of the consortium, it is composed by the Principal Investigators of all Parties and is chaired by the Coordinator. The role of the GA is to define the strategy and make all formal decisions for the CoE. As from the Consortium Agreement, it meets at least twice a year. Permanent invited members are representatives of Unimore and CSIC, and the Cnr MAX Management Team.

2. The **Work-Package Leaders Committee (WP-Exec)** is a newly established governing body, a small and agile board for the execution of the Project that monitors the progress of the WPs individually and jointly, reports to and is accountable to the General Assembly. The WP-Exec is formed by the leaders of each WP and chaired by the Coordinator, a deputy, or a person from the Management Team. The WP-Exec meets at least quarterly, but extraordinary meetings could be held upon request of any partner. Chair of the WP-Exec, appointed by the General Assembly in February 2023, is **Andrea Ferretti,** Cnr.

WP n.	Title	Leader	Node	Deputy	Node
WP1	Lighthouse Applications for Materials Science	Stefano Baroni	SISSA	Daniel Wortmann	FZJ
WP2	Exascale workflows and extreme data	Nicola Marzari	UBremen	Alberto Garcia	CSIC
WP3	Technical challenges towards exascale and post-exascale	Fabio Affinito	CINECA	Jan Jona Javorsek	IJS
WP4	Co-design & technology exploitation	Lubomir Riha	IT4I@VSB	Kaveh Haghighi Mood	FZJ
WP5	Training & Community engagement	Daniele Varsano	CNR		
WP6	Communication, exploitation, and dissemination	Alex Argemi	ICN2		
WP7	Management	Luisa Neri	CNR		

Fig. 3. Composition of the WP-Exec.

3. The **Coordinator** is the legal entity acting as the intermediary between the Parties and the Granting Authority and coordinating the execution of the decisions of the General Assembly. In addition to its responsibilities as a Party, the Coordinator performs the tasks assigned to it as described in the Grant Agreement and the Consortium Agreement. The Coordinator (flanked by the Technical Project Manager) also manages MAX external relations, especially building and maintaining strategic relationships within the ecosystem, coordinates the external action of the CoE, its presence at meetings and events, and strictly collaborates to develop the communication lines. The Coordinator is **Elisa Molinari,** Cnr.

4. The **WP Committees** are agile coordination and executive boards within each WP: each one is formed by the Leaders and co-leaders of each WP and of the related Tasks.

5. The **Technical Project Manager** is an operational entity that flanks the Coordinator in MAX external relations within the HPC ecosystem, operates in close connection with WP leaders and continuously assesses that work tasks and allocated budget are used according to the proposal and the plans.

6. The **Software Technical Board** (STB) gathers a representative of each code supported in the consortium and is the institutional body to exchange technical and software engineering best practice among the different development teams (notably, each team/code has its own software quality assessment process and internal procedures concerning SW repositories, CI/CD, SW releases, etc). Moreover, the STB allows us to technically discuss strategies and opportunities concerning software development. Since WP1 is devoted to codes, the STB is led by the Leader of WP1 and typically meets during the WP1 meetings.

7. The **Management Team** supports the work of the Coordinator and of the Consortium as a whole for the day-to-day management of the project and is set in the Coordinator's node. The management team is in charge of supporting activities of the governing bodies, ensuring an efficient internal communication; overseeing reporting deadlines and quality control; collecting and (e-)archiving the project documents. The management procedures are aimed at the effective implementation of the work plan and the successful completion of MAX deliverables and milestones.

Work performed in the first 12 months:

1) The **General Assembly (GA)** met, in person, twice:
- at the Kick-off meeting in Modena (IT) on February 22, 2023
- at the periodic Meeting in Barcelona (ES) on October 17, 2023

In the first GA meeting, a series of permanent invited additional members to the GA were appointed (from Affiliated Entities and Management Team); roles in the governing boards of the CoE were assigned; a list of events to attend were chosen. Relations with existing bodies such as the Castiel2 CSA and the HPC3 (HPC Centres of Excellence Council) were discussed and planned. At the second GA, held during the Project Meeting in Barcelona, the Coordinator presented the Collaboration Agreement drafted by Castiel2, and received the support from all partners for its development. Actions and plans to undertake collaborations with the other CoEs and National Competence Centres (NCCs) networks were discussed and agreed upon.

2) The **Work-Package Leaders Committee** met on September 13, 2023 to discuss the status of WP activities in view of the upcoming MAX meeting (Barcelona, October 16-17, 2023); first report period (M12) and review.

4. MAX Management and Management Team

MAX management is ensured by WP7, led by the Coordinator's node CNR Nano, with the collaboration of all partners.

Objectives

- Establishing, implementing, managing, and reporting all main aspects of the CoE as a whole;
- ensuring close interaction and coordination among all the WPs for a fruitful collaboration and transversal project implementation;
- fostering the effective cooperation and integration of all the teams and activities;
- ensuring the financial, legal and administrative project management;
- defining the standards, the tools and the procedures for the internal communication;
- monitoring the KPIs progress and the risk assessment;
- controlling of the internal and formal submission deadlines for the correct and on time delivery and reporting of the project achievements;
- contributing to the training, communication, and dissemination activities;
- taking care of institutional relations with different actors (e.g., the national Competence Centres);
- fostering and promoting inclusivity- and gender-aimed actions.

Structure

The WP7 Management is led by the WP leader, **Luisa Neri,** and the Management team. It refers to the Coordinator **Elisa Molinari** and Co-PI **Andrea Ferretti**.

- *WP7 Leader*: **Luisa Neri.**

  She coordinates the management staff, and flanks the General Assembly, the WP-Exec and the Coordinator from the managing point of view, in close connection with the other WP leaders, the nodes financial offices and the EC. She boasts long experience in management activities, both in the previous MAX phase and in several EU H2020 projects, national projects and regional ones.

- *Management Team:* composed by Cnr Nano staff that has gained experience from the previous project phases. The management team composition has changed along the projects duration and now include: **Maria Bartolacelli** and **Susanna Cavicchioli,** MAX Technical Secretariat, **Daniele Varsano,** liaison with WP5 and WP6, **Maddalena Scandola,** press office, **Nicola Spallanzani,** software development and developer teams manager, **Maria Grazia Angelini,** administration, all belonging to the Cnr Nano staff. Further support and contributions are coming from the staff of Cnr Nano or other units.

5. WP7 Activities

Several activities have been performed since the beginning of the project (01/01/2023). Below a description of the work performed following the structure: 1. a box (blue border) with the provision of the Description of Actions (DoA) divided by task; 2. a paragraph with the description of the concrete implementation realised so far.

5.1 T7.1 Task description

T7.1: Establishing and supporting the CoE governance *(months 1-48, Task leader: CNR, Partners: All)*

This task will take care of setting-up and supporting the operation of MAX governing bodies, as well as their connection with all WPs. This task overviews the activities of the GA and the WP-Exec. As a dashboard for the governing bodies and the management, this task will revise and finalise the list of KPIs and related targets defined in this proposal (see WP description), and will perform KPI monitoring and updating. The task will also coordinate the monitoring, and necessary revision of the Risk management list.

Outputs: Boards organised and running; Management of schedule; yearly periodic update of KPIs.

Performed work and main results achieved

1. ***Consortium Agreement discussion and definition***: the Consortium Agreement was signed by all partners within month 2. No changes have occurred since.
2. ***Organization of the Kick-off meeting***, February 21 and 22, 2023 in Modena (IT) hosted by Cnr Nano ***and related General Assembly***[1]. The details of the General Assembly are described at point 2. CoE Governing Bodies.

[1] http://www.max-centre.eu/max-kick-meeting-february-21-and-22-2023-modena-it

Fig. 4. Group photo of the Kick-off Meeting - February 21 and 22, 2023 in Modena (IT) @AGO Fabbriche Culturali Modena | FEM - Future Education Modena.

3. ***Organization of the first project meeting*** | MAX Project Meeting - October 16 and 17, 2023 in Barcelona (ES) hosted by ICN2 ***and related General Assembly***[2].

Fig. 5. Group photo of the MaX Project Meeting - October 16 and 17, 2023 in Barcelona (ES).

4. ***KPI updating and monitoring:*** with the collaboration of all partners: the WPs discussed internally the definition and the quantitative and qualitative measurements of each KPI. The list of KPIs is given at the end of this document.

[2] http://www.max-centre.eu/news/max-project-meeting-october-2023

5. ***Risk monitoring****:* a detailed risk list has been defined in the Grant Agreement, with the definition of the WPs involved and some measures of risk-mitigation. Risk management will be an integral part of the entire project lifecycle. The management followed the evolution of all WP activities in the first 12 months and will continue for the rest of the project duration. After the first 12 months of the project, the management team has also updated the likelihood of some risks (e.g. risks 5, 7, 8 have been raised to level "medium", risk 13 has been lowered to "medium", and risk 16 has been added anew). The management will also support the WPs in the implementation of contingency actions if and when needed. Notably, the management team has been observing the evolution of the European HPC ecosystem and the related MaX activities,

Risk nr	Description	Work Package Nr	Proposed Mitigation Measures
1	The conflicting requirements of different hardware, middleware, and software stacks deployed on EuroHPC systems by different vendors may delay the delivery of a unified codebase. (medium risk)	WP1	T1.1 and T1.2 will prioritise the performance optimisation and the timely delivery on each architecture. T1.3 will, if needed, solve code-base unification issues in the long term (milestones at M30 and at M48)
2	The delivery of future EuroHPC systems may require unexpected adaptations of the programming models deployed in our software, or the adoption of entirely new ones. (low risk)	WP1	WP1 and WP3 will work in close collaboration to promptly adapt the programming model. If needed, targeted training events will be organised with WP5 to update the developers.
3	Inadequacies of early releases of the software stacks, especially for the new architectures, may cause sub-optimal initial results in performance improvement. (medium risk)	WP1	The modularisation of the codes will allow us to explore and exploit different competing solutions.
4	Some workflows demand scheduling and resource management technologies that are not yet available. (medium risk)	WP3, WP2	A trade-off between scheduling efficiency and data persistence can be reached.
5	Access to appropriate allocations for demonstrators is not forthcoming (low risk => medium risk)	WP2	A scaled-down version of the workflow implementation can be run on available systems.
6	Programming open standards features are not immediately integrated in vendor-specific compilers and/or tools (medium risk)	WP3	We will implement ad-hoc workarounds for specific features or we will address open solutions for compilers and tools (e.g. the GNU toolchain).
7	The availability of allocated computing resources is not sufficient to run benchmarks and proof-of-concepts (low risk => medium risk)	WP3	We will rely on in-kind contribution of resources from the computing centres that are partners of the project.

8	Some of the prototype platforms (EPI, EUPEX, EUPilot) will not be available on time. (low risk => medium risk)	WP4	We will seek alternative platforms which will be in terms of hardware parameters and used technologies as close to the prototype platforms as possible.
9	Production HPC systems will not allow us to tune hardware parameters of the compute nodes. (high risk)	WP4, WP3	HPC systems at IT4I@VSB have already enabled this tuning knob for the research group involved in this project. Also CINECA systems enable this. The experimental and prototype platforms, such as EUPEX, in most cases enable this.
10	The planned training offer is insufficient with respect to the requests. (low risk)	WP5	Organisation of online schools that will exploit a seamless cloud environment to hold modern online hands-on sessions (virtual computer laboratory). High-quality recordings of lectures and relevant training material will be offered in an ad-hoc developed web repository for training.
11	There is limited interest in the education and training offered by the CoE. (low risk)	WP5	Focused actions in event advertising in collaboration with WP6, forthcoming CSA and National Competence Centres. Training events organised in collaboration with (e.g., at the premises of) National Competence Centres.
12	Users and stakeholders not responsive to the selected communication & dissemination channels (medium risk).	WP7, WP6	Multiple different media and communication & dissemination strategies will be used, making the action flexible.
13	New pandemic (COVID-19 or similar) outbreak, and consequent limitations to travelling, hiring, networking, in-person activities, training. (medium-high risk => medium risk).	WP7, WP6	For collaborative, training, networking activities: expert usage of online tools to hold virtual meetings, training or communication events. To mitigate difficulties in hiring, we will try to activate an increased effort of staff or remote hiring and training of new personnel, according to institutions' rules.
14	Risk 1- Potential users of MaX codes not ready to take advantage of the new EuroHPC architectures (medium/high)	WP7, WP6, WP5	Adopt ad hoc training initiatives aimed at building basic HPC skills in the community of potential users (of electronic structure methods in materials science). Expand the introductory part of MaX training events, with special attention to cross fertilisation with HPC competences (e.g.incl heterogeneous architectures). Coordinate with CASTIEL2, nCCs, and HPC centres.

15	Slow adoption of MaX codes by end users (including industry) (low/medium)	WP7, WP6, WP5	Work with Castiel2 and nCCs to coordinate engagement and training actions; Design dedicated training schemes for industry (eg. on premises training); Develop dedicated turn-key solutions within appropriate agreement (industry).
16	Access to the CoE budget share from the member state is difficult (medium risk)	WP7	Coordinate with the member state institutions connected to the EuroHPC funding scheme. Worst case scenario: apply for further funding.

Table 1: Critical risks & risk management strategy.

5.2 T7.2 Task description

T7.2: Operational management of the CoE *(months 1-48, Task leader:* ***L. Neri*** *– CNR, Partners: All)*

This task ensures the management of the daily activity of MAX, as well as the implementation of the goals defined by the governing bodies. The responsibilities of this task include: • Deliverable production and quality control; • Reporting and support to liaison with EuroHPC; • Financial management and reporting; • Ensuring effective internal communication; • Collaborating with the communication staff.

Performed work and main results achieved

1. ***Day-to-day coordination of the project activities and of the secretariat activities:*** an intense internal communication has been established since the beginning of the project. An informal starting meeting has been held on December 13, 2022 to involve the new partners and inform them about MAX procedures and fundamental workflows.

2. ***Monitoring of WPs thematic work and deadlines respect***: the management team supports the WP Leaders in the organisation of the periodic meetings of their WPs, singularly and collectively. It also monitors the meetings calendar and progress. The Scientific WPs (1-4) meet on a monthly basis (see Fig. 6).

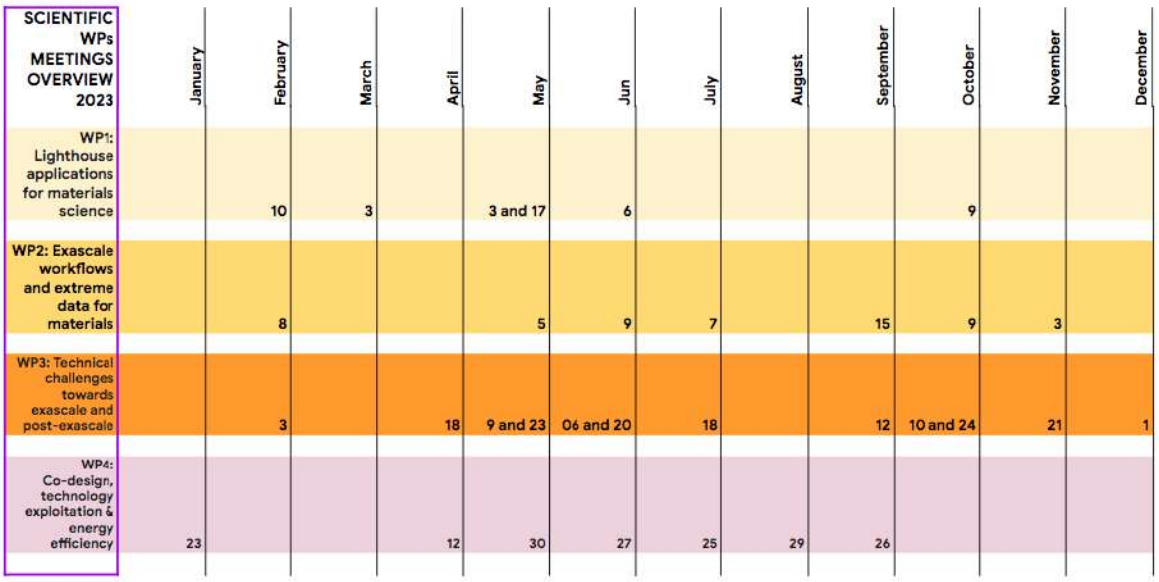


Fig. 6. WPs 1-4 meetings calendar 2023.

3. ***Monitoring of the internal periodic report***: detailed instructions have been shared with the partners regarding the continuous reporting activities needed.

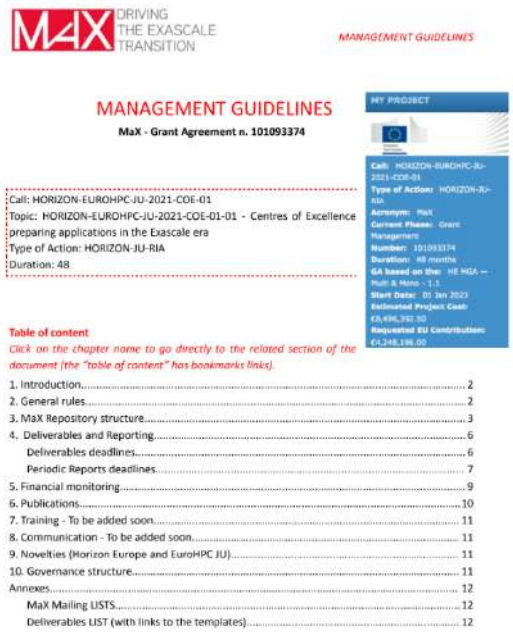
4. ***Definition of the guidelines, internal procedures and templates*** for deliverables and other project documents.
   - Organization of a detailed calendar, for the collection of inputs, reports and meetings. To ease the partners' activities, the respect of the deadlines and to make available all the links and useful information at once and in a handy way, the management team prepared and shared, from the very beginning of the project, a **"SINGLE ENTRY POINT" document**.
   After the successful experience of the second phase, the document has been improved and completed. It contains different kinds of information:

   - all the fundamental/official/general information to correctly report (grant Number, reporting periods, logos and disclaimers for the dissemination and communication activities, acknowledgement for the scientific publications, etc…);
   - the information related to the Consortium structure (PIs list, WP leaders and deputies list, mailing lists);
   - the calendar with all the deadlines (internal and official ones) divided into future and past ones;
   - the deliverables list, an overall picture and a list with links for every deadline (M6-M12-M18-M24-M30-M48);

- the detailed instructions for the correct periodic reporting activity.

Thanks to a presentation of the management system that was given at the kick-off meeting, and thanks to the availability of a written instructions document, all the management processes went on pretty smoothly also with the new partners.

The definition and sharing of written **GUIDELINES for Management procedures (see Annex 1)** constitutes a great improvement of the present MAX phase compared with the previous ones. The guidelines are a handy tool for all the partners to cope with the different deadlines and activities


MAX DRIVING THE EXASCALE TRANSITION

MANAGEMENT GUIDELINES

MANAGEMENT GUIDELINES

MaX - Grant Agreement n. 101093374

Call: HORIZON-EUROHPC-JU-2021-COE-01
Topic: HORIZON-EUROHPC-JU-2021-COE-01-01 - Centres of Excellence preparing applications in the Exascale era
Type of Action: HORIZON-JU-RIA
Duration: 48

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Fig. 7. Management Guidelines cover.

In addition to the Management guidelines, the Management team collaborated with the WP5 “Training & community engagement with the HPC ecosystem” leader to draft training specific guidelines that are available in MAX Drive.

5. ***Overall legal, administrative and financial management*** (budgeting and financial reporting, distribution of the EU financial contribution among partners, support to partners regarding financial and administrative issues and duties). The Management Team was in charge of the Grant Agreement draft, and relevant interactions with the JU; of the Consortium Agreement draft and finalisation; of collecting and overseeing the financial development of the CoE (especially national contributions and IKOP monitoring).

6. ***Reorganisation of the MAX internal repository*** and an internal IT infrastructure using Google Apps. The internal IT infrastructure, available since the second edition of MAX, has been re-organized in a more user-friendly way based on experience and feedback from partners. The Consortium used:
   - A Google Drive repository organised in thematic folders;
   - A Google Calendar (with different sub-calendars) for internal deadlines, official ones and meetings overview (WP meetings, general meetings - Kick-off, project meetings, review meetings, etc…) + relevant events for the community;
   - Google accounts have been created for all the project participants;

- Google Groups have been created to facilitate internal communication;
- Google Meet is the channel used for periodic formal and informal meetings.

Furthermore we set up MAX software repositories on GitHub, GitLab, DockerHub, and defined other communication channels (MAX-centre Slack).

7. In collaboration with all partners and WPs, WP7 is also planning, organising, and implementing ***transversal activities*** in close collaboration with WP5 "Training & community engagement with the HPC ecosystem" and WP6 "Communication, exploitation, and dissemination".

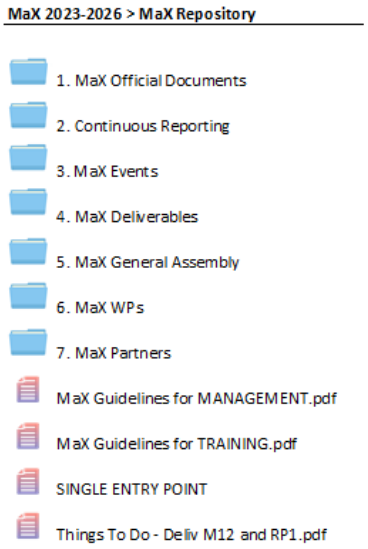


Fig. 8. MaX Repository (Google Drive) overview.

5.3 T7.3 Task description

T7.3: Ensuring optimal interfaces and interactions with the broader European ecosystem, especially with Competence Centres and with EuroHPC projects, infrastructures and environment (Collaboration) (months 1-48, Task leader: ***E. Molinari*** *– CNR, Partners: All)*

This task promotes and manages the interactions and collaborations of MAX as a whole with the European ecosystem. It also coordinates and supports the technical interactions to be deployed by all the other pertinent WPs. More specifically, WP7 will ensure:

• Interfacing on policy and technical issues; setting up dedicated working groups, when needed, to address issues raised within the European ecosystem;
• Interfacing with Competence Centres and EuroHPC supercomputing consortia to sustain training and common initiatives, especially for countries within the EuroHPC JU that are currently developing and advancing their HPC infrastructure and ecosystem;
• Interfacing with national initiatives within Europe;
• Working with the other CoEs and the future CSA against the fragmentation of European HPC activities in applications; coordinate with complementary CoEs to share best practices and actions;
• Interfacing and collaborating with communities and organisations in the computational materials research domain (e.g., CECAM, Psi-k).

Performed work and main results achieved

As in the previous phases MAX aims at being one of the driving forces within the European HPC ecosystem. In order to do so, we actively pursue effective interfaces with the main components of the ecosystem both on policy and technical issues.

In these early months, MAX members have taken part in a number of events, as detailed below.

Fig. 9. A view of the main MAX synergies and partners in the European HPC and materials domain ecosystems.

5.3.1 EuroHPC JU

MAX participated and actively collaborated in the initiatives of the Euro HPC Joint Undertaking:

1. **CoEs meeting** held on February 8, 2023. An informative meeting regarding the call HORIZON-EUROHPC-JU-2021-COE-01, with an overview on call details, reporting and reviews procedures, collaboration needed, and an open session for question and answer.
2. [EuroHPC Summit Week 2023] held in Gotheborg (SE) March 20-23, 2023. **Elisa Molinari, Andrea Ferretti, Claudia Cardoso** (CNR), **Daniele Cesarini** (CINECA), **Daniele Gregori** (E4), **Estela Suarez** (FZJ), and **Ivan Carnimeo** (SISSA) contributed to the meeting in different ways as reported below.

Tuesday 21.03.2023 | EuroHPC User Opportunities Day

Parallel Session 01 (14.30-16.00) - Available EuroHPC Computing Resources: How to Access Them? : talk by **Claudia Cardoso** (CNR Nano).

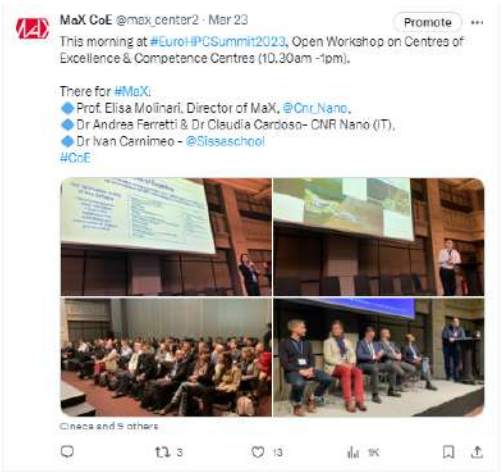
Parallel Session 02 (16.30-18.00) - User Communities' Scientific Expectations in the Exascale Era: Examples from Chemistry, Biology, Astrophysics and Space Physics3: talk by **Elisa Molinari** (CNR Nano, Unimore and MAX Director) + round table on the topic.

Wednesday 22.03.2023 - EuroHPC JU Scientific Challenges Day

Scientific Developments in HPC & Energy Efficiency: Showcasing the Latest Scientific Innovation in HPC and Energy Technologies (9.00-9.45): talk by **Daniele Cesarini** (CINECA).

Parallel Session 02 (14.30-16.00) - Spotlighting EuroHPC Projects: Innovations for next generation of HPC applications: talk by **Daniele Gregori** (E4 Computer Engineering).

Parallel Session 03 (14.30-16.00)- Emerging Technologies for HPC in Europe: A Conversation on Latest Developments in Emerging Technologies: contribution of **Estela Suarez** (FZJ).



Thursday 23.03.2023 - EuroHPC Ecosystem Communities Day

10.30-13.00 Open Workshop: Centres of Excellence & Competence Centres - **Elisa Molinari** (CNR Nano, Unimore and MAX Director), **Andrea Ferretti** and **Claudia Cardoso** (CNR Nano), **Ivan Carnimeo** (SISSA).

Euro HPC User Day on December 11, 2023 in Brussels (BE). **Elisa Molinari** has chaired the Computational

Chemistry parallel session and **Ivan Carnimeo** (SISSA) has been invited as speaker in the Computer Science session.

5.3.2 CASTIEL2

MAX is involved in the activities of CASTIEL2, the Coordination and Support Action (CSA, Grant Agreement n. 101102047) that promotes the harmonisation and reinforcement of endeavours undertaken by the National Competence Centre (NCC) and Centre of Excellence (CoE) initiatives on a pan-European scale. We share the common objective to facilitate collaborations among NCCs and CoEs, as well as within our respective communities, to maximise our influence on the European High-Performance Computing (HPC) landscape and user base. CASTIEL2 is organising this common effort nurturing networks, promoting interaction, and identifying areas of synergy. It has defined several working packages with specific tasks, and representatives and deputies from all the CoEs are requested to attend.

MAX representatives are involved in all the CASTIEL2 WPS respectively:

- WP2 “NCCs/CoEs Networking and Mapping of Competences, Codes and Services” - **Nicola Spallanzani** (CNR) and **Andrea Ferretti** (CNR) - deputy;
- WP3 “Training, Twinning, Mentoring”: **Daniele Varsano** (CNR) and **Maria Bartolacelli** (CNR) - deputy;
- WP4 “NCCs, CoEs and Industry Interaction”: **Luisa Neri** (CNR) and **Nicola Spallanzani** (CNR) - deputy;
- WP5 “Awareness, Impact and Outreach” **Alex Argemì** (ICN2) and **Virginia Greco** (ICN2) - deputy.

Competence Centres and CoE Advisory Board. A joint board elected by NCCs and CoEs representatives in September 2023, in order to advise CASTIEL2 on suitable actions for the best possible collaboration between projects and help align the strategy to best support the CoEs with joint activities on the CASTIEL2 side.
The WP7 leader **Luisa Neri** has been elected as a deputy for Topic 1 (HORIZON-EUROHPC-JU-2021-COE-01) along with Niclas Jansson (CEEC) and Marisa Zanotti (SPACE). Members elected from Topic 2: R. Apostolov (BioExcel 3), D. Hoppe (HIDALGO 2); deputies J. Biercamp (Esiwace 3), T. Esposti Ongaro (Cheese-2P). Eight more members have been elected from the NCC side.
So far, the CaB met on October 5, 2023 and December 12, 2023.

Collaboration Agreement (COLA). As foreseen in the Grant Agreement, Section 1 Consortium: Beneficiaries, Affiliated Entities And Other Participants, Article 7 — Beneficiaries "(...) If required by the granting authority (see Data Sheet, Point 1), these arrangements must be set out in a written collaboration agreement with the participants of the other action or, if the consortium is the same, as part of their consortium agreement, covering for instance:
- the internal organisation and decision making processes; - the areas where close collaboration/synchronisation is needed (e.g., on management of outputs, common approaches towards standardisation, links with regulatory and policy activities, common communication and dissemination activities, sharing of information, access to background and results, etc.); - settlement of disputes; - liability, indemnification and confidentiality arrangements between the beneficiaries in both actions."
WP7 leader **L. Neri** has followed the draft of the COLA on MAX side, continuously interacting with CASTIEL2 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.

CI/CD Collaboration Task. One of CASTIEL2 collaboration tasks involves the active contribution of supporting CoEs' codes to a shared continuous integration and application deployment (CI/CD) platform. This involvement includes the implementation of automated testing, potentially utilising a Special Access scheme in collaboration with CASTIEL2. The goal is to ensure this process is applied across all EuroHPC JU systems. During the first year, operational meetings were organised regarding this activity, and we actively participated in them. We responded to requests to test the available CI/CD procedures on at least one EuroHPC machine and provided our feedback. The shared platform for CI/CD is currently in the creation phase, and we will continue to respond to action requests as they are proposed to us. Our representatives for this activity are **Jan Jona Javoršek** (as leader of task 4 of MAX's WP3 concerning a similar activity) and **Barbara Krašovec and Nicola Spallanzani** as deputies.

MAX representatives attended all the different regular meetings, with significant active contributions:

TRAINING 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

INDUSTRY 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 CASTIEL2:

- **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.

Fig. 10. MaX Tweet on CASTIEL2 Kick-off attendance (on the left) and a group photo.

- Attendance to the NCCs-CoEs meeting organised online by CASTIEL2 on April 18-19, 2023. The meeting gave NCCs and CoEs the chance to better get to know each other and discuss future collaborations. It was also a further opportunity to understand the role of

CASTIEL2 and its different WPs. MAX presented its work in the session dedicated to "older" CoEs.

Additional details on all these collaborations are offered in deliverable D7.4.

5.3.3 EUMaster4HPC

Several partners of MaX belong to the EuMaster4HPC Consortium where they play important roles. Here we point out that MaX as a CoE is actively contributing in liaising the EuMaster4HPC with the CoEs ecosystem, e.g. by spreading information and promoting awareness within HPC3, and with the materials domain ecosystem. The goal for the EuMaster4HPC is taking advantage of the CoEs experience (e.g. mentoring, stage hosting, use of available training materials etc); conversely, the CoEs can especially gain from a fruitful interaction with the education strategies and with students, also in view of possible future hiring. MaX coordinator Elisa Molinari has directly contributed to the promotion activities. She also actively participated in an interesting informal EuroHPC-EuMaster4HPC women and diversity meeting (Fig. 11).

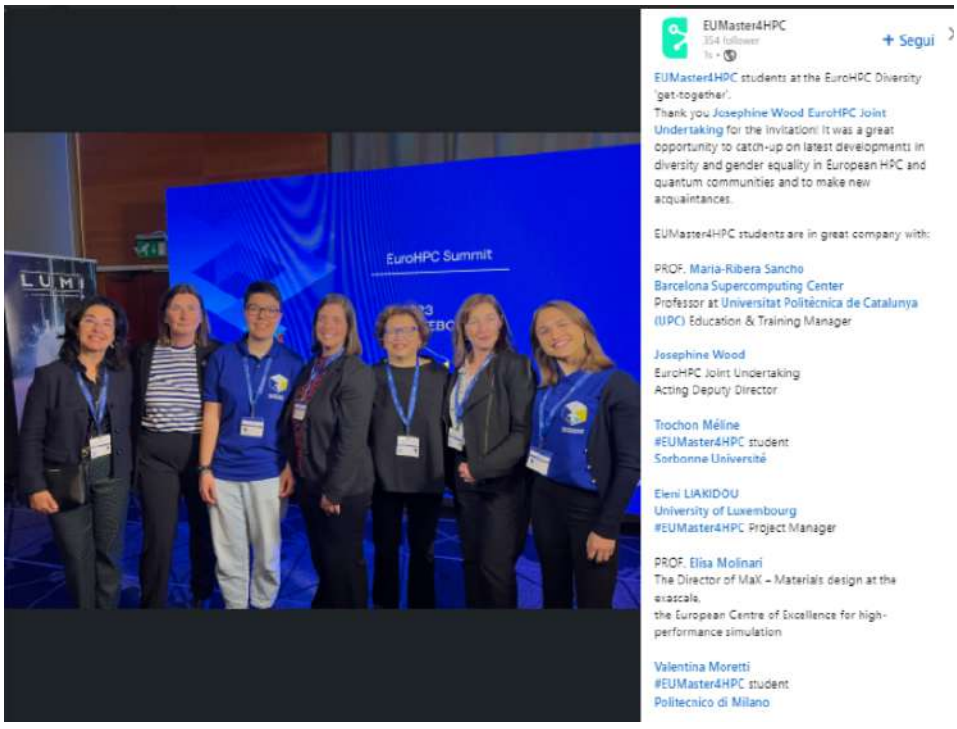


Fig. 11. Group photo with EUMaster4HPC students and partners at the EuroHPC Diversity get-together, where Molinari of MaX enjoyed interesting conversations especially with the master students. The get-together, organised by Jo Wood during the EuroHPC Summit week, was a very successful opportunity for networking.

5.3.4 International activities: the EU-Japan collaboration

MaX partners continue to participate in several international collaborations and events of great relevance, which are not supported by the EuroHPC JU but greatly contribute to our own advancements as well as global impact.

In the present context we only report on the MaX activities concerning the EU-Japan collaboration, since it directly involves the EU and the EuroHPC JU. The EU-Japan Digital Partnership was launched in May 2022 during the 29th Japan-EU summit in Tokyo. An important component concerns extreme-scale supercomputers and hybrid quantum HPC systems in Europe and in Japan, and as such involves the collaboration with EuroHPC. Materials science were recognized as one of the key application domains of relevance for the Partnership:

"53. Both sides should exchange information regarding optimising HPC applications of common interest for future generations of supercomputing platforms/architectures (pre-exascale, exascale, post-exascale, hybrid Quantum-HPC). The starting point could include applications related to biomedical, material science, seismic/tsunami and/or weather and climate modelling."[3]

Elisa Molinari as MaX Director was invited, together with other CoE representatives, to establish and structure the collaboration on applications, and for this she has co-organized working sessions and innumerable informal meetings. She has paid special attention in engaging the communities within and beyond the partnerships of MaX and other CoEs.

In 2023 the main event was the **EU-Japan virtual Workshop on High Performance Computing**, held on-line on 25 January 2023 (see the Agenda in Fig. 12). MaX has actively contributed to shaping the event. We have collected information about possible collaborations with Japan from the broader communities, in order to ensure effective interactions and participation. Elisa Molinari presented the results and the materials applications ecosystem of EuroHPC and joined the discussion with the Japanese partners throughout the workshop.

EU-Japan Workshop on High-Performance Computing
25 January 2023
8:30-11:45 CET / 16:30-19:45 JST (VIRTUAL)

AGENDA

8:30-8:40	Welcome	Thomas Skordas, Deputy Director General DG CNECT + Naohito Kimura, Deputy Director General, Research Promotion Bureau - MEXT (TBC)
8:40-9:00	Digital Partnership - HPC focus	Gustav Kalbe, Director C - DG CNECT + Taku Kawahara, Director, Office for the Promotion of Computing Science - MEXT
9:00-11:00	• Materials (40 min) ○ Elisa Molinari (University of Modena and Reggio Emilia) and Edouard Audit (CEA); Takahito Nakajima (Riken) and Yoshitaka Tateyama (National Institute for Materials Science) • Biomedical (40 min) ○ Erik Lindahl (Stockholm University) and Alfonso Valencia (Barcelona Supercomputing Center); Yuji Sugita (Riken) and Florence Tama (Riken) • Climate/Weather/natural events (40 min) ○ Joachim Biercamp (DKRZ) and Jorge Macias (University of Malaga), Masaki Satoh (University of Tokyo) and Satoru Oishi (Riken)	
11:00-11:10	Presentation of EU specific HPC focused action to support the Digital Partnership	Leonardo Flores, DG CNECT
11:10-11:20	Discussion on access to EU-Japan systems	Gustav Kalbe – Kengo Nakajima, Vice-Director of R-CCS (tbd)
11:20-11:40	Q&A - discussions	All
11:40-11:45	Conclusions and wrap-up	Gustav Kalbe+ Taku Kawahara

Fig. 12. Agenda of the EU-Japan virtual Workshop on High Performance Computing.

[3] https://digital-strategy.ec.europa.eu/en/news/eu-japan-summit-strengthening-our-partnership

Most recently, after a EuroHPC call was launched to promote collaborative projects with Japan, MaX has worked with other CoEs to structure a proposal through a consortium, led by CEA, that can ensure effective cooperation and impact on HPC science and technologies in Europe. The proposal, named Hanami, was successful; the project will start in

February 2024 and last for 3 years. It brings together leading research teams in HPC both in Europe and Japan (the partnership includes 14 European and 10 Japanese research organisations, see Fig. 13). Key expertise will be pooled in pre- and exascale systems, and the research will support organisations and industrial stakeholders involved in the developing HPC technologies for extreme-scale architectures.

The project aims to port applications in the domains identified by the EU-Japan Digital Partnership on extreme-scale supercomputers and hybrid quantum HPC systems in Europe and in Japan. All partners in the consortium support the common objective to strengthen and improve the HPC ecosystem in Japan and Europe through the co-design of applications and sharing of information and expertise around HPC. MaX is contributing to Hanami goals and actions in the application domains of materials science, and co-leads the corresponding work package and related collaborations. Several MaX partners and codes will be directly involved, including Siesta (P. Ordejon, ICN2), BigDFT (Genovese, CEA), Fleur (S. Bluegel, FZJ) and Yambo (D. Varsano, CNR).

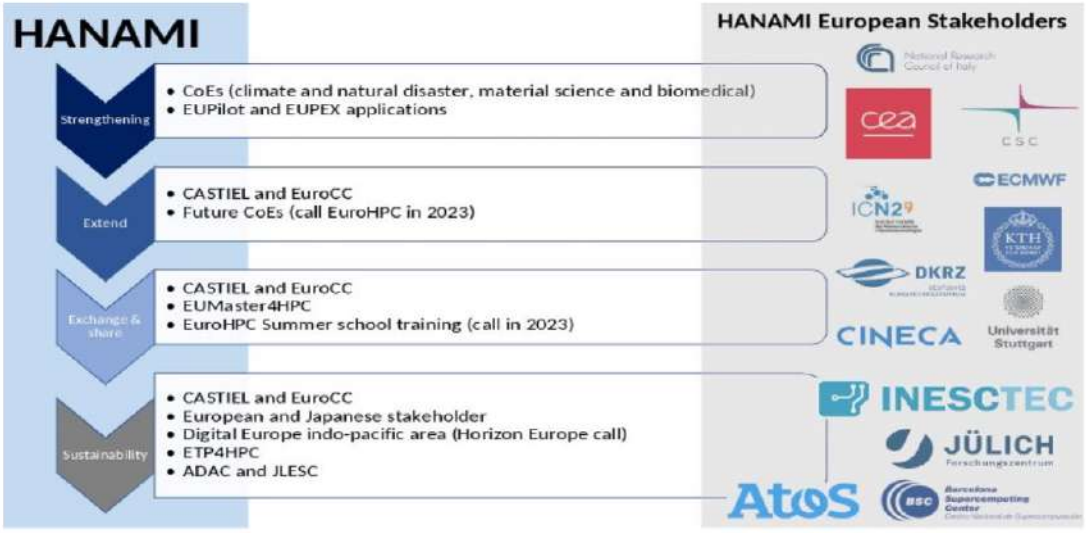


Fig. 13. Structure and European stakeholders of the Hanami project. Several MaX partners and codes contributed to design the materials science pillar and its collaboration with the European and Japanese ecosystems.

5.3.6 Collaborations on technical issues with the EuroHPC ecosystem and HPC Consortia

MaX has continued to work within the EuroHPC ecosystem in order to design common strategies to address key technical challenges. The specific outcomes are part of the relevant deliverables produced by WP1-WP5. Here we summarise some of the collaborative events to which we have contributed.

Nicola Spallanzani (Cnr) was one of the invited speakers of the "MPI and OPENMP in scientific software development - online training" organised by NCC Netherlands on June 12, 2023[4].

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

Laura Bellentani (CINECA) and **Nicola Spallanzani** (Cnr) participated in 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, 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[5].

Laura Bellentani (CINECA) and **Fabrizio Ferrari Ruffino** (Cnr) were invited speakers at the December 2023 appointment of the ECP SOLLVE - OpenMP Teleconferences. Monthly calls are organised so that ECP application teams may share their OpenMP experiences with the community and bring any related issues or concerns to the attention of the compiler developers and OpenMP language committee members. They presented a talk on "OpenMP Offload Quantum ESPRESSO" on December 1, 2023[6].

5.3.7 Prace

[4] https://eurocc-netherlands.nl/calendar/mpi-and-openmp-in-scientific-software-development/
[5] https://eventi.cineca.it/en/hpc/introduction-leonardo-hpc-cluster-users-and-developers/bologna-20231027
[6] https://www.openmp.org/events/ecp-sollve-openmp-monthly-teleconference/

At present Prace is collaborating with the EuroHPC JU in various ways, but its future evolution is still under debate. Meanwhile, Prace has recently organised a "Workshop to update of the PRACE Scientific and Innovation Case for Computing in Europe" at Sorbonne University in Paris (FR) on October 20, 2023, and **Elisa Molinari** gave an invited keynote lecture as a prominent scientist in condensed matter physics and director of the MAX CoE.

5.3.8 Lhumos

Lhumos (Learning Hub Materials Simulation) is a web-based archive for the training and dissemination material (videos, notes, presentations) for simulations and modelling of materials, and beyond, via high-performing computing preparing for the exascale transition. This ad-hoc web repository was established and developed in the previous MAX project, as a common effort by MARVEL, CECAM, MAX, and MultiXscale, and will be launched with a live webinar on January 15, 2024. The repository was advanced during 2023 and will be continuously enhanced in the coming months.

Fig. 14. Banner of the upcoming webinar.

We will work in close collaboration with other European digital and HPC initiatives as they develop, in order to ensure the most effective contribution of MAX to the EuroHPC JU ecosystem. Lhumos will serve as a platform for training in high-performance computing and simulation and modelling for materials and other related fields. Users will have access to recorded lectures and a wealth of supporting training materials to enhance their understanding and skills in these domains.

5.3.9 Policy activities in the materials domain: the Advanced Materials 2030 and the Batteries 2030+ Initiatives

We mention in particular the Advanced Materials 2030 Initiative[7] (AMI2030), which aims to set up a pan-European multi-sectoral accelerator for the design, development and uptake of sustainable advanced materials towards a circular economy. Thanks to their engineered functionalities, Advanced Materials play an important –often critical– role in the green and digital transition while simultaneously reinforcing Europe's strategic sovereignty. A large effort is

[7] https://www.ami2030.eu/

thus being developed by many European (mostly industrial) stakeholders and member states in order to shape a Strategic Materials Agenda that can contribute to the next EU Framework Programs.

Elisa Molinari was involved in advancing some aspects of the Strategic Materials Agenda (SMA), some of which closely related to MaX ideas and background. She took part in the workshop: "From the Materials2030Manifesto towards a Strategic Agenda for advanced materials'' (held on January 11, 2023 online) and in other informal discussions. As a matter of fact, the combination of "digital" and "materials" is now recognized as a key component of the SMA in several important ways.[8]

The Battery2030+ initiative has witnessed a significant participation of MaX, especially through BIG-MAP[9] –the Battery Interface Genome - Materials Acceleration Platform–, one of its main projects centred on the HPC and AI convergence in materials design for future batteries. In 2023 MaX has been working on the next BIG-MAP strategies and their integration into the EuroHPC supercomputing and applications ecosystem. Marzari, Ordejon, Molinari and others participated in several informal meetings hopefully leading to strengthened collaborations.

5.3.10 Community activities in the materials domain

MaX continues to collaborate very actively with networks, organisations and institutions that structure the scientific community in the materials domain in Europe and globally. In 2023 we have held some coordination meetings and started to plan future collaborative initiatives:

- Psi-k network[10], especially on the opportunities for schools/workshops and MaX participation in the 2025 Psi-k conference (Blugel, Marzari, Molinari, Ordejon and others)
- CECAM[11], especially on the opportunities for webinars and workshops, as well as the Lhumos initiatives (Blugel, Marzari, Molinari, Varsano and others)
- ICTP[12], especially for collaborations around international activities, possible hackathons/workshops, as well as the Master in High Performance Computing (Cavazzoni, DeGironcoli, Affinito, Molinari and others)

[8] https://www.ami2030.eu/wp-content/uploads/2023/04/Ami2030-Dossier-2.pdf
[9] https://www.big-map.eu/
[10] https://psi-k.net/
[11] https://www.cecam.org/
[12] https://www.ictp.it/

- ETSF[13], especially for collaborations in webinars and possible meetings (Varsano and others).

Some joint initiatives have already taken place, more will be organised in the future and will be reported in the appropriate deliverables.

5.4 T7.4 Task description

T7.4: Implementation, assessment, revision and promotion of gender policies within the CoE (months 1-48, Task leader: CNR, Partners: All)

This task will take care of the gender equality and diversity equality balance within MAX, coordinating and assessing activities planned and implemented by partners and WPs (especially WP5 & WP6) to help fill the gender gap and improve inclusivity, promoting initiatives with and towards broader communities (e.g., specific training initiatives, communication actions addressed to women or young students).

Performed work and main results achieved

This task was introduced in order to take into account the challenges that gender and diversity policies present for research institutions, academia, science in general, and the HPC world in particular. Though this project does not plan to develop specific gendered innovations, its consortium as a whole, and as individuals, pays great attention to promote a safe, equal, and inclusive environment for its personnel. It fosters positive actions for the raising of awareness, for the empowerment of women in leading roles, for the widening of STEM and HPC female audiences.
All this is done by each partner within its institutional tasks, not necessarily linked to MAX, but in complete agreement with its view. On the other hand, several actions have been undertaken by MAX, especially in training and communication.

1. Gender-policy survey. First of all, members of the management team (**Bartolacelli, Cavicchioli,** and **Neri**) have started to collect data on the partner institutions' activities, such as their Gender Equality Plans, their actions devoted to positive and inclusive policies, communication actions, hiring policies, and so on. The survey will lead to the drafting of streamlined guidelines for gender-policy rules within MAX. This will be revised by all partners and presented by M18.

2. Communication and awareness-raising activities.

[13] https://www.etsf.eu/

- **Initiatives for the International Day of Women and Girls in Science (Feb 11, 2023).** Social campaign on MAX channels with both original posts and re-posting of partners initiatives;

- **Elisa Molinari** was an invited speaker for the webinar **"From Women's eyes"** organised by CECAM in the framework of the International Day of Women and Girls in Science[14]. Online, February 10, 2023.

[14] https://www.cecam.org/lecture-details/womens-eyes-2023

- **European Researchers' Night 2023 in Modena (IT)**. Cnr Nano organised the event **"To Become a Scientist, I Start" – Life and Adventures of Two Young Researchers in the World of Nanoscience**, an informal conversation about the world of nanoscience with a female scientist's perspective. **Caterina Chiari** and **Claudia Cardoso** (Cnr, actively involved in MAX CoE), shared their journey as young researchers in cutting-edge science fields such as ultrafast electron microscopy and material design. During the event, they discussed their career choices, the challenges they have faced, and the most exciting moments of their research, engaging in a dialogue with **Vincenzo Grillo** on the topic of gender equality in science. The event took place in room D, San Geminiano Area, via San Geminiano, 3, Modena.[15]

Fig. 15. Claudia Cardoso at European Researchers' Night 2023.

- MAX supported the realisation of the video **"300x100: protagoniste per la ricerca"**, showcased during the celebration of the centenary of CNR National Research Council (IT) in Rome (November 18, 2023). The video presented the leading role of female scientists at Cnr and celebrated the social campaign #womenatCNR[16] that presented for one year the activity of almost 300 Cnr scientists. MAX supported the campaign and the video for it shows positive role models and the fundamental role of women in science.

[15] https://twitter.com/max_center2/status/1707745764053553337
[16] https://centenario.cnr.it/evento/300x100-protagoniste-per-la-ricerca/

Fig. 16. Elisa Molinari in “300x100” video.

3. Training activities. Gender issues are paramount for our training activities, as presented in the Training and Education Programme (D5.1 M6). In the *executive summary*, it was highlighted how the training activities focus on the plan for specialised training, education, and support in computational materials science, with a strong emphasis on best practices for developing and running MAX lighthouse codes on HPC machines. Throughout each action, special attention will be given to young individuals and women in research and technology, ensuring an inclusive and gender-balanced representation among the lecturers and instructors. Building upon previous successful experience, the MAX-supported events will adhere to well-defined guidelines to ensure measurable impacts in terms of participant numbers, women's participation, and feedback from attendees.

   In section *"Introduction and Objectives,"* it was emphasised that the training activities stipulate that all MAX initiatives should be guided by principles of inclusiveness and gender balance, in fact these are the main evaluation parameters that are collected as a result of the events organised and promoted by MAX.
   The table below provides an overview of statistics for five MAX training schools conducted in the year 2023, where it can be seen that 62 out of 228 participants were women, which represents 27%, as for tutors, 6 out of 34 were women, i.e. 18%, and finally 10 out of 67 women were lecturers, which is equivalent to 15%.

	PARTICIPATION STATS 2023											
	Name of the school	Dates	Location	Total applicants	Total participants	Women participating	Academia	Industry	total tutors	Women tutoring	total lecturers	Women lecturing	User's satisfaction
1	Quantum espresso targeting accelerator ICTP	27-28/02/2023	Trieste ICTP, Italy		18	4	5	8			8	1	
2	All electron DFT with fleur	8-12/05/2023	Juelich, Germany	32	11	1	11	0	4	0	11	0	5 (all voted for "very likely" on "How likely are you to recommend this tutorial/school to a colleague?")
3	Ab initio many-body perturbation theory: from equilibrium to time-resolved spectroscopies and nonlinear optics	22-26/05/2023	Rome, Italy	88	39	10	39	0	4	0	16	5	4.64/5
4	Advanced Quantum ESPRESSO school: Hubbard and Koopmans functionals from linear response	28/8-01/09/2023	Pavia, Italy	180	41	12	40	1	10	1	21	2	8.5/10
5	First steps with SIESTA: from zero to hero	2-6/10/2023	Online	156	119	35	118	1	16	5	11	2	4.63/5.00

Fig. 17. Training statistics 2023.

6. KPIs

A detailed list of *key performance indicators* (KPIs) is given in the Table below. These KPIs have been taken from the DoA and updated. In particular, KPIs 3.1, 3.2, 3.3, 3.4 were added on request of the PO, and now replace our previous KPIs corresponding to WP3 (mostly overlapping with the newly requested ones). Notably, the identified targets may be subject to amendments according to the development of software and hosting architectures (this is in particular the case of K3.1-K3.4, which make explicit reference to the CI/CD infrastructure which is currently under development in collaboration with CASTIEL-2) .

While in the present report we are not able to provide an assessment of the KPIs at M12, the results will be presented and discussed in the first Periodic Report.

Deliverable D7.3: Report on the setup of the MAX CoE

KPI n.	Description of KPI	WP	Measurement procedures	Target M12	Target M18	Target M24	Target M30	Target M36	Target M42	Target M48
K1.1	Improvement in the intra-node performance of MAX codes (e.g. measured in terms of time-to-solution; see K4.3 for energy efficiency).	1	At M12 Select a few HPC clusters of reference: (eg: VEGA, Leonardo for NVidia cards, LUMI-G for AMD, Jupyter or MareNostrum5 for Intel...). Tests defined with WP3	INTERMEDIATE TARGETS: linear fraction of M48 targets						Increase in TTS 15 %for NVIDIA, 35 % for AMD w.r.t. M18 or M24. (Other possible target: increase memory efficiency 20 % for NVIDIA)
K1.2	Improvement of the parallel efficiency of MAX light-house codes on selected EuroHPC machines (e.g. Leonardo, LUMI, MareNostrum-5, or the exascale machines) wrt a baseline (set at the beginning of the project or when the machines are deployed for production).	1	At M12 Select a few HPC clusters of reference: (eg: VEGA, Leonardo for NVidia cards, LUMI-G for AMD, Jupyter or MareNostrum5 for Intel...). Tests defined with WP3	INTERMEDIATE TARGETS: linear fraction of M48 targets						25%
K1.3	Number of new ports of MAX codes and libraries to different hardware architectures.	1	Evaluation from the release reports	3	5	8	10	12	14	15 new ports [2 for each code/libs (eg AMD, Intel)]
K1.4	Number of new code functionalities enabled to run on massively parallel heterogeneous systems.	1	Evaluation from the release reports	1	2	4	6	8	9	10
K2.1	Number of exascale workflows designed	2	At M12 we have a deliverable: Report on the design, architecture, implementation and development plan for exascale workflows, according to T2.1. The boldface is ours, understanding that the design work will be ongoing through M48. Since there are a number of fronts to coordinate, each with their own timeline, it is not likely that we can actually finish any design before, say, M24.	0	0	1	2	3	4	6
K2.2	Size of the largest HPC partitions exploited by the exascale workflow infrastructure built by MAX	2	Size in units of nodes (targets to be updated if needed when new machines are deployed)	128	128	256	256	512	512	1024
K2.3	Number of exascale workflows demonstrated on EuroHPC machines	2	This is linked to K2.2. All the workflows designed should probably be demonstrated soon afterwards, i.e. the 'design' should really mean 'implementation'.	0	0	1	2	3	4	6
	Average percentage % coverage of EuroHPC systems	3	Includes breakdown by partition (e.g. CPU, GPU)	40%	40%	60%	70%	80%	90%	100%
K3.1	No of applications deployed to JU systems incl. breakdown by partition (e.g. CPU, GPU).	3	All MAX codes will be deployed to JU systems, on both cpus and gpus partitions	intermediate targets: 5 codes * Target % coverage * Number of available partitions						All MAX codes will be deployed to JU systems, on both cpus and gpus partitions
K3.2	No of EUROHPC systems supported by application incl. breakdown by partition (e.g. CPU, GPU).	3		Intermediate targets: No of available EuroHPC partitions * Target % coverage						
K3.3	No of errors (failed deployments/ regression tests) identified through common platform.	3		intermediate targets are all equal to Target M48						5-10 bugs/year (1-2 bugs per code per year)
K3.4	Average time from failed application test to deployment of corrected application.	3	The time needed to solve a problem depends on the type of problem, it can range from a few days to months	intermediate targets are all equal to Target M48						2 months
K4.1	Number of co-design actions/analysis performed using co-design vehicles from/relevant for MAX codes	4	Number of co-design reports (report = one apps/mini-apps on one vehicle)	4	6	7	10	11	12	14
K4.2	Number of advanced hardware solutions tested using MAX codes, libraries, or mini-apps	4	Number of advanced hardware solutions where MAX kernels/mini-apps/codes are deployed and benchmarked in terms of time to solution.	3	5	6	7	8	9	10
K4.3	Improvement on energy efficiency (e.g., in terms of energy-to-solution) of MAX flagship codes/libraries	4	Improvement of energy consumption on selected hardware platforms with hardware parameters tunning when compared to default runtime/system settings (without tuning).		Report on energy consumption evaluation		Energy to solution improved by **10%** using static tuning			Energy to solution improved by **15%** using dynamic tuning
K5.1	Number of people trained in MAX training events (in terms of person-training days), including gender statistics.	5		750	1130	1500	1880	2250	2630	3000
K5.2	Number of collaborative actions for the HPC ecosystem	5		2	4	6	8	10	12	14
K6.1	Total number of invited talks to conferences and schools plus total number of publications	6	K6.1 will be measured through detailed tracking of the talks provided by members of the MAX network. This will be done via an established information flow on the Google Drive platform where the project results are internally reported. Publications will be measured using a dual approach: the manual information flow established within Google Drive, but also through programmed alerts on Web of Science. This will allow us to detect and semi-automatically include new publications that mention MAX in their acknowledgements.	Invited talks: 4; Publications: 30		Invited talks: 8; Publications: 60		Invited talks: 12; Publications: 90		Invited talks: 16; Publications: 120
K6.2	Total number of people in the MAX network (social media, registered to the newsletter, event participants)	6	K6.2 will be reported using the analytics tools of MAX's social networks (LinkedIn, Twitter, and YouTube), the project's Newsletter management tool, which will be relaunched around M10, and tracking within the project's Google Drive intranet of the impact of events organised under the auspices of MAX.	Social Media Followers: LinkedIn (900), Twitter (1500), YouTube (550); Newsletter subscribers: 800; Event participants: 400		Event participants: 800		Event participants: 1200		Social Media Followers: LinkedIn (1800); Twitter (3000), YouTube (1000); Newsletter subscribers: >1000; Event participants: 1600

7. Conclusions

MAX activity in M1-M12 has been quite intense due to the setting-up and launch of the new consortium, different rules to follow in EuroHPC JU, many requirements for reporting and exciting challenges for the development of the foreseen actions. A great amount of work has been devoted to actions in collaboration with the CSA Castiel2, to play a fruitful role in the European ecosystem of CoEs and NCCs.

No major issues have been faced within the consortium, all partners have actively participated in its activities, and we intend to continue this way in the upcoming months.

MANAGEMENT GUIDELINES

MaX - Grant Agreement n. 101093374

Call: HORIZON-EUROHPC-JU-2021-COE-01
Topic: HORIZON-EUROHPC-JU-2021-COE-01-01 - Centres of Excellence preparing applications in the Exascale era
Type of Action: HORIZON-JU-RIA
Duration: 48

Table of content

Click on the chapter name to go directly to the related section of the document (the "table of content" has bookmarks links).

The MaX Management guidelines are produced by Luisa Neri and Maria Bartolacelli, Cnr Nano Modena (April 2023)

1. Introduction

We report here the MANAGEMENT GUIDELINES, as explained by Luisa Neri, WP7 Leader, during our Kick-off Meeting in Modena.

2. General rules

For info or requests related to WP7 - MANAGEMENT - write to:

- the management team's members name.surname@max-centre.eu
- always put management@max-centre.eu in cc

We use a Common G-suite working space, accessible with your MaX account name.surname@max-centre.eu (please ask again if you missed the email with the instructions to set your account and password).

Please follow our suggestions and requests listed below:

1. Enter the MaX G-drive space: **Repository MaX 2023-2026**

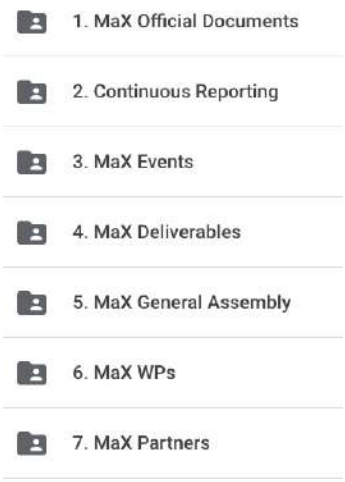
   SUGGESTION: the repository is in the "Shared with me" items, you may add a shortcut to your drive to be able to find the MaX repository easily (right click on the repository/drop down menu/add shortcut to Drive) →

2. Add MaX shared calendar to your calendar portfolio.
3. Check periodically the mailing lists and inform us about:
   - Job openings
   - New collaborators
   - Updates in general
4. Become familiar with MaX tools.
   Refer to the SINGLE ENTRY POINT file for dates, deadlines, useful info in general and don't hesitate to contact the management team for doubts.
5. Become familiar with MaX social media:
   Website http://www.max-centre.eu/
   Twitter @max_center2
   LinkedIn company/max-centre/
   YouTube youtube/channel/MaX Centre eXascale
6. Organize regular periodic WP meetings (ideally on a monthly base)
7. Fill in continuously the spreadsheets:
   - PUBLICATIONS
   - EVENTS

For more info:

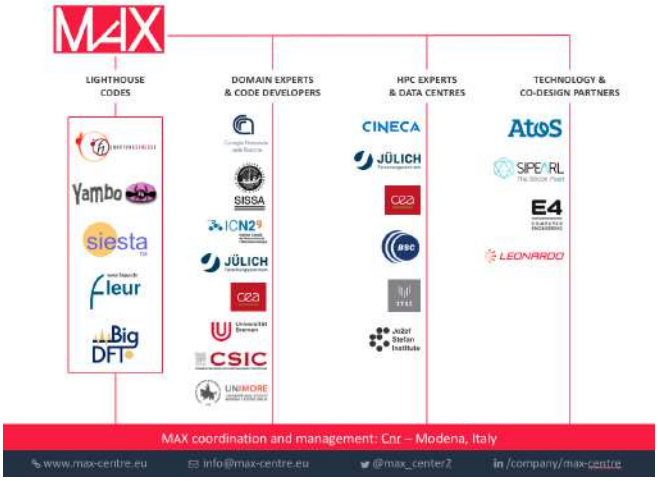
MaX Repository | MaX Calendar | SINGLE ENTRY POINT

3. MaX Repository structure



MaX Repository contains now 7 folders: Official docs, Continuous reporting, Events, Deliverables, General Assembly, WPs, and Partners. →

1. **"1. MaX Official documents"** contains all the official docs submitted and signed sofar: the Submitted Proposal and its evaluation, the Grant Agreement, the Consortium Agreement (in progress), the pre financing letter as well as some communication tools: MaX Logo and MaX Brand identity manual + the graphic scheme of MaX partnership. ↓



We will upload here all the official documents coming from the EC and the EuroHPC JU regarding the project: notifications, amendments, review reports, etc…

2. **"2. MaX Continuous Reporting"** contains:

- the spreadsheet of the PUBLICATIONS → please add here all the publications related to MaX (with a formal acknowledgement to MaX - Grant n. 101093374) and complying with the Open Access rules required by Horizon Europe.
- "OPEN ACCESS GUIDELINES 2023", for your convenience we added here a google doc with some Open Access rules and the standard acknowledgement.

Open Access in Horizon Europe

Open science: open access to scientific publications

The beneficiaries must ensure open access to peer-reviewed scientific publications relating to their results. In particular, they must ensure that:

- ✓ at the latest at the time of publication, a machine-readable electronic copy of the published version, or the final peer-reviewed manuscript accepted for publication, is **deposited in a trusted repository** for scientific publications
- ✓ **immediate open access is provided** to the deposited publication via the repository, under the latest available version of the Creative Commons Attribution International Public Licence (CC BY) or a licence with equivalent rights; for monographs and other long-text formats, the licence may exclude commercial uses and derivative works (e.g. CC BY-NC, CC BY-ND) and
- ✓ information is given via the repository about any research output or any other tools and instruments needed to validate the conclusions of the scientific publication.

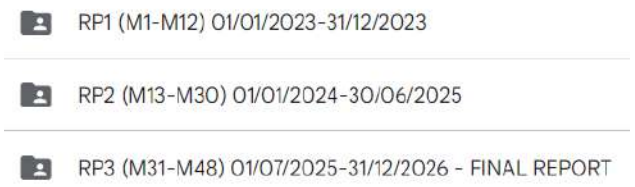
Beneficiaries (or authors) must retain sufficient intellectual property rights to comply with the open access requirements.

Metadata of deposited publications must be open under a Creative Common Public Domain Dedication (CC 0) or equivalent, in line with the FAIR principles (in particular machine-actionable) and provide information at least about the following: publication (author(s), title, date of publication, publication venue); funding statement (see Article 17); grant project name, acronym and number; licensing terms; persistent identifiers for the publication, the authors involved in the action and, if possible, for their organisations and the grant. Where applicable, the metadata must include persistent identifiers for any research output or any other tools and instruments needed to validate the conclusions of the publication.

Only publication fees in full open access venues for peer-reviewed scientific publications are eligible for reimbursement.

From Art.17 - EU Grants: HE MGA — Multi & Mono: V1.0 DRAFT – 25.02.2021

In the folder there are 3 sub-folders with the templates of the periodic reports and data collection related to each reporting period.



Furthermore you may find there the file "Visiting researchers": please fill it with information about researchers visiting your labs during the whole project duration.

3. **"3. MaX Events"** → is meant to collect all events attended or organized under the MaX acknowledgement. Please add your organized or attended events in the file "Complete list of MaX3 events" and let us know about it. WP6 will use these info to promote your event. In case of organized events, a contact person will be needed, someone who will attend it and provide pictures and texts for social media coverage.
   In this folder the main info related to each event organized or attended by MaX partners, pictures, presentations, participants list, etc… are collected.

4. **"4. MaX deliverables"** contains all the templates of the deliverables divided per WP as wella as an overview of deliverables per month and per partners.

5. **"5. General Assembly"** contains all documents and minutes related to the meetings and decisions of the GA.

6. **"6. WPs"** is a dedicated repository for each WP. Each Wp has a dedicated room store where all the files it wants to share with working group and the management team. →

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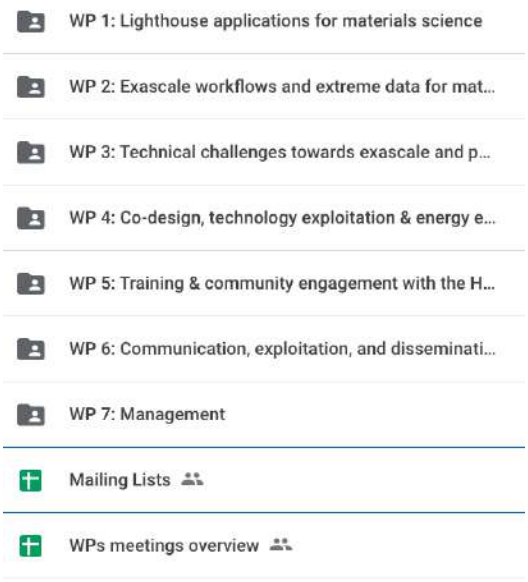
In the folder there are two additional files, see the screenshot on the right: o a G-sheet with the mailing lists and G-sheet with the WPs meeting overview.



7. **"7. MaX Partners"** is an additional working space divided per partner. Each partner can use its folder to save documents and files.

4. Deliverables and Reporting

MAX STARTING DATE **JANUARY 1, 2023**
MAX END DATE: **DECEMBER 31, 2026**

General rules for deliverables and periodic reports:

1. *Internal deadline is 1 month before the official deadline (both for deliverables and periodic reports)*. At this date it is important to share with the management team a draft of the deliverables or a contribution to relevant sections of the periodic report.

Deliverables deadlines

Month	***Internal deadline***	***Official deadline***
M6	May 31, 2023	June 30, 2023
M12	November 30, 2023*	December 31, 2023
M18	May 31, 2024	June 30, 2024
M24	November 30, 2024*	December 31, 2024
M30	May 31, 2025	June 30, 2025
M36	November 30, 2025*	December 31, 2025
M48	November 30, 2026*	December 31, 2026

*****This deadline at the end of November is of utmost importance, as the official deadline is at the very end of the year and we need to be ready well beforehand, in order to allow the Management team and those in charge to review everything on time.

2. Inform WP Leaders and management on setbacks/problems/delays
3. Answer promptly and helpfully to calls for contributions and info requests
4. Continuous and timely report (Drive)
    - Scientific activities
    - Financial activities (national call - IKOP)
    - Comm-diss, training, gender…
    - KPIs (table 3.1k of the Grant Agreement). WPs are in charge of their own KPIs.

KPI number	Description of KPI
K1.1	Improvement in the intra-node performance of MAX codes (e.g. measured in terms of time-to-solution; see K4.3 for energy efficiency).
K1.2	Improvement of the parallel efficiency of MAX light-house codes on selected EuroHPC machines (e.g. Leonardo, LUMI, MareNostrum-5, or the exascale machines) wrt a baseline (set at the beginning of the project or when the machines are deployed for production).
K1.3	Number of new ports of MAX codes and libraries to different hardware architectures.
K1.4	Number of new code functionalities enabled to run on massively parallel heterogeneous systems.
K2.1	Number of exascale workflows designed
K2.2	Size of the largest HPC partitions exploited by the exascale workflow infrastructure built by MAX
K2.3	Number of exascale workflows demonstrated on EuroHPC machines
K3.1	Number of profiling and benchmarking campaigns
K3.2	Number of advanced programming model solutions analysed and demonstrated as PoC/mini-apps
K3.3	Percentage of European HPC clusters MAX lighthouse-code are deployed for production.
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 platform.
K3.7	Average time from failed application test to deployment of corrected application.
K4.1	Number of co-design actions/analysis performed using co-design vehicles from/relevant for MAX codes
K4.2	Number of advanced hardware solutions tested using MAX codes, libraries, or mini-apps
K4.3	Improvement on energy efficiency (e.g., in terms of energy-to-solution) of MAX flagship codes/libraries.
K5.1	Number of people trained in MAX training events (in terms of person-training days), including gender statistics.
K5.2	Number of collaborative actions for the HPC ecosystem
K6.1	Total number of invited talks to conferences and schools plus total number of publications
K6.2	Total number of people in the MAX network (social media, registered to the newsletter, event participants)

Periodic Reports deadlines

RP1 (REPORTING PERIOD 1): 1/01/2023 - 31/12/2023 (M1-M12)
RP2 (REPORTING PERIOD 2): 01/01/2024 - 30/06/2025 (M13-M30)
RP3 (REPORTING PERIOD 3): 01/07/2025 - 31/12/2026 (M31-M48)

The formal deadline for each periodic report is: 60 days after the end of the reporting period. REMEMBER that our internal deadline will be set much earlier because we are supposed to send to the PO and the reviewers the draft of the Periodic Report Part B - with some tables related to person months, expenses and justifications of the deviations - 15 days before the review meeting to let them read all the report and the last deliverables). The review meeting is typically scheduled within the 60 days after the end of the reporting period.

RP	***Internal deadline***	***Official deadline***
1	TBD	29/02/2024
2	TBD	31/08/2025
3	TBD	28/02/2027

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We collect the info in the Periodic Report files:

RP1 (REPORTING PERIOD 1): 1/01/2023 - 31/12/2023 (M1-M12)

WP1-4 RP1

WP5-7 RP1

RP2 (REPORTING PERIOD 2): 01/01/2024 - 30/06/2025 (M13-M30)

WP1-4 RP2

WP5- 7 RP2

RP3 (REPORTING PERIOD 3): 01/07/2025 - 31/12/2026 (M31-M48)

WP1-4 RP3 - Final

WP5-7 RP3 - Final

What you are expected to do:

- If you are a **WP leader**, lead the drafting of your WP section. An introduction is needed and then a description task by task. Contributions by all partners must be added in the description and in the section "main achievements''. Ask the partners for contributions.
  It is important to point out (i) any deviations from DoA; (ii) activities done with other WPs.
- If you are a **partner,** be ready to collaborate and contribute to all tasks and WPs in which you have worked by providing contents and main achievements.
  The shared files of the periodic reports will be available in the Continuous Reporting folder in the drive.
- If you are a **PI**, please complete with your administrative office the Raw Financial data tables: person months and budget (this data will be inserted in point 5.2 "Use of resources" of the report).
  Please note: the official financial data have to be handled within 60 days from the end of the reporting period, but it is fundamental that we present a financial overview, as accurate as possible, in the final report - usually handed in before the Review-, to discuss with reviewers significant deviations.

5. Financial monitoring

Constantly inform the management team about:

- National calls and co-funding status
- IKOP

Furthermore:

- submit any issues!
- when asked for informal financial reporting (usually for the period report we need rough data about financial aspects, over/under spending and related justifications) - please answer! *Please note that the formal financial data will follow a different road and are needed within 60 days after the closure of the reporting period.*
- read carefully the GA for new rules - *art.* ***6.3 Ineligible costs and contributions***
  "The following costs or contributions are ineligible: …
  (e) other:
  (i) costs or contributions for activities that do not take place in one of the eligible countries or target countries set out in the call conditions - unless approved by the granting authority."

6. Publications

Acknowledgement for publications

MaX "MAterials design at the eXascale" co-funded by the European High Performance Computing Joint Undertaking (JU) and participating countries under grant agreement No. 101093374.

Please inform the management team about ongoing publications: we would like to make visible all the scientific publications on the MaX website.
Please fill the spreadsheet PUBLICATIONS adding all the info related to all the publications related to MaX (with a formal acknowledgement to MaX - Grant n. 101093374) and complying with the Open Access rules required by Horizon Europe.

We need the support of the authors to define different communication pieces throughout MaX digital outlets (example here 1 Tweet, 1 LinkedIn post, 1 tailored news piece for the website). The communication team will ask for a brief text for the newspiece containing the overall background description of the scientific challenge tackled in the publication, some details on the research team that carried that out, the role and/or added value of MaX (e.g. codes used), the most relevant outcomes and some hints on the work methodology, which innovative sides of the publications you would like to point out, take-home message easily shareable with scientists not expert in the field + if any, specific images from the publication to be used/attached in the news and persons, authors and/or organizations to be tagged (both on LinkedIn and Twitter).
If possible, it could also be helpful having few lines for creating the tweet, with keywords that should stand out in the message (if any specifically).

7. Training - To be added soon

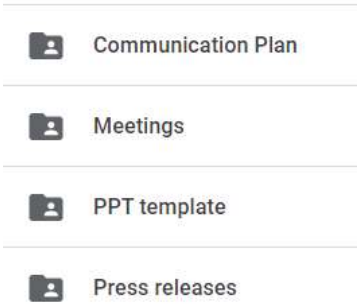
You will receive specific guidelines for WP5 meant to harmonize the MaX offer and to fulfill the EC recommendations.

In the google drive, inside the folder WP5, you already have some sub-folders related to past and future schools/workshops.

8. Communication - To be added soon

You will receive specific guidelines for WP6.

In the google drive, inside the folder WP6, you already have some useful files →



9. Novelties (Horizon Europe and EuroHPC JU)

1. **Collaboration task**: compulsory task to work with Castiel2 and other CoEs, NCCs and the CSA on technical issues.
2. **Gender equality and diversity equality balance within MaX** (esp. WP5 & WP6):
   We will make a report of the existing situation and we will need to collect info from your institutions and examples of good practices. Please provide the name of a contact person, collaborate, and communicate all related information from your institution.

10. Governance structure

- **The General Assembly (GA)**
- **The Work-Package Leaders Committee (WP-Exec)**
- **The Coordinator**

The General Assembly (GA): meets at least twice a year, always invite the affiliated entities (CSIC & Unimore) to General Assembly meetings, and invite management team members to General Assembly meetings.

The Work-Package Leaders Committee (WP-Exec): meets at least quarterly, Andrea Ferretti (Cnr) has been appointed Chair of WP Leaders Committee.

During the first informal General Assembly attendants agreed to meet twice a year as a consortium, one in person (in autumn) and one online (in spring) to check the status of advancement of the project.

Annexes

MaX Mailing LISTS

Active mailing lists:
MaX All members | max@max-centre.eu
MaX General Assembly | general-assembly@max-centre.eu
MaX Principal Investigators | pi@max-centre.eu
MaX WP Leaders| wp-leaders@max-centre.eu
MaX Management | management@max-centre.eu
MaX Communication | communication@max-centre.eu
wp1@max-centre.eu
wp2@max-centre.eu
wp3@max-centre.eu
wp4@max-centre.eu
wp5@max-centre.eu
wp6@max-centre.eu
wp7@max-centre.eu
If you want to check who is inserted in each mailing list please check here (mailing lists updated periodically, please control the date in the first row!). Ask the management team for changes, additions or modifications!

Deliverables LIST (with links to the templates)

Deliverables M6 (30/06/2023)
D1.1 First report on software architecture and implementation planning - SISSA
D5.1 Training and Education Programme - CNR
D6.1 MAX communication, exploitation, and dissemination Plan - ICN2
D7.1 Collaboration plan with definition of common objectives and activities including milestones - CNR
D7.2 Data Management Plan - UBREMEN

Deliverables M12 (31/12/2023)
D1.2 First release of MAX software: report on performed and planned refactoring - FZJ
D2.1 Exascale workflow design - CSIC
D3.1 Interim report on performance analysis of MAX software - CINECA
D4.1 Advanced Technologies Monitor - E4
D7.3 Report on the setup of the MAX CoE - CNR

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D7.4 Update of collaboration plan (month 12) - IJS

Deliverables M18 (30/06/2024)

D1.3 Second report on software architecture and implementation planning - SISSA
D2.2 Code interoperability - SISSA
D3.2 Interim report on programming models solutions for exascale efficiency - SISSA
D4.2 Report on energy consumption evaluation - IT4I@VSB

Deliverables M24 (31/12/2024)

D2.3 Report on the exascale metascheduler - IT4I@VSB
D3.3 Interim report on system middleware for workflows and resilience - IJS
D5.2 First report on MAX training events - CNR
D6.2 Impact Assessment Report, mid-term version - ICN2
D7.5 Interim report on MAX management - CNR

Deliverables M30 (30/06/2025)

D1.4 Second release of MAX software: report on lighthouse codes' deployment at exascale - CEA
D2.4 First report on exascale workflow infrastructure and demonstrators - LEONARDO
D2.5 FAIR data, reproducibility, and provenance - CINECA
D4.3 First Co-design report - SIPEARL
D6.3 MAX communication, exploitation, and dissemination Plan – Final version - ICN2
D7.6 Second update of collaboration plan (M30) - BSC
D7.7 Revised Data Management Plan - UBREMEN

Deliverables M48 (31/12/2026)

D1.5 Third official release of MAX software - CEA
D2.6 Final report on the exascale workflow infrastructure and demonstrators - UBREMEN
D3.4 Final report on performance analysis of MAX software - CINECA
D3.5 Final report on programming models solutions for exascale efficiency - SISSA
D3.6 Final report on system middleware for workflows and resilience - IJS
D4.4 Final Co-design report - ATOS
D4.5 Final report on advanced technology exploration - FZJ
D4.6 Report on energy consumption optimisation - IT4I@VSB
D5.3 Final report on MAX training events - CNR
D6.4 Impact Assessment Report – Final version - ICN2
D7.8 Final report on MAX management - CNR
D7.9 Final report of collaboration plan - BSC

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