D10.5

Final report on CoE governing bodies activity

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D10.5 Final report on CoE governing bodies activity

Executive Summary

The deliverable D10.5 "Final report on CoE governing bodies activity" of the MAX materials at the Exascale project presents the activity of Tasks *T10.1 Establishing and supporting the CoE governance* and *T10.2 Operational management of the CoE*. In the following, the activities of the governing bodies, of the management team, the assessment of Key Performance Indicators (KPIs), and an analysis of the risk management is given. The overall activity of the Centre of Excellence has proceeded smoothly in the 46 months, for the management experience in large projects and the proactive collaborations of all partners.

1 Final report on CoE Governing Bodies (Task 10.1)

As defined in the DoA (section B.3.2) and agreed upon by the partners in the Consortium Agreement (art. 6.1) the organisational structure of this Consortium is composed by the MaX Director, the General Assembly (the official governing body), the Executive Committee, the Software Quality Management Board, and the International Advisory Board.

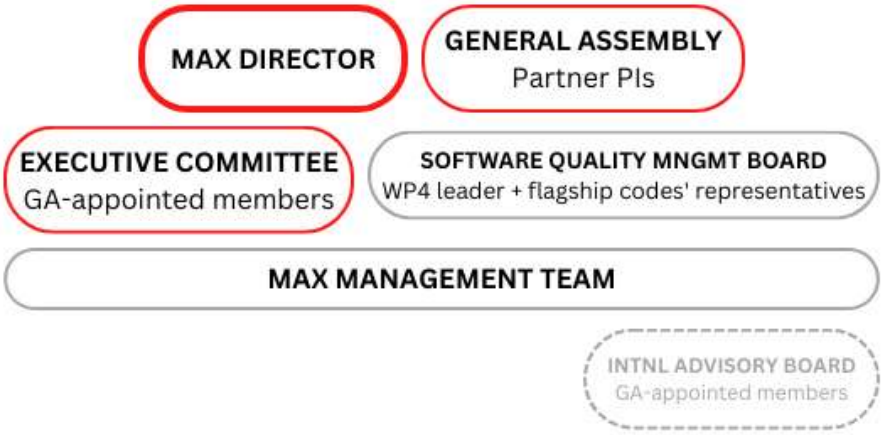

Fig 1. MaX management structure.

The activity of the Boards is briefly described below. To begin with, it is important to state that no pitfalls or obstacles have been met during the life of the project as far as the boards are concerned. The partners have all collaborated to the boards and have properly flanked the Coordinator in steering the consortium, from both a scientific/technical and an administrative/management point of view. A strong collaboration has been developed among WPs, that has led to a common effort in developing all the assigned tasks, but also in building and promoting a strong MaX identity. This is highly demonstrated, e.g., by the common effort done in WP7-10, the most transversal WPs.

As a further example, we point out the great participation to the Psi-K conference in Lausanne (22-25/08/2022), which saw the collaboration of all attending partners to the common activities, the booth and the special MaX events (see xxx for details).

Fig 2. MaX group picture at the Psi-K conference, Lausanne (August 2022).

1.1 The General Assembly

The **General Assembly (GA)** is the official governing body of the CoE. It is composed by the PIs of all participating teams plus some invited members with no voting rights and coordinated by the Director. It has the task of taking strategic and formal decisions concerning the Centre.
The members who have attended the meetings are
Participants attending with voting rights (Partners' PIs)

- CNR. Elisa Molinari
- SISSA. Stefano Baroni
- ICN2. Pablo Ordejón
- Jülich. Stefan Blügel
- CEA. Thierry Deutsch
- EPFL. Nicola Marzari
- UGent. Stefaan Cottenier
- CINECA. Carlo Cavazzoni; Fabio Affinito
- BSC. Stephan Mohr; José Maria Cela; Julio Gutierrez
- ETHZ. Joost VandeVondele
- E4. Fabrizio Magugliani

- ARM. Filippo Spiga; Conrad Hillairet
- ICTP. Ivan Girotto
- Trust-IT. Silvana Muscella

Invited participants without voting rights

- Andrea Ferretti (CNR) - Executive Committee Coordinator
- Daniel Wortmann (Jülich) - WP2 Leader
- Daniele Varsano (CNR) - WP8 Leader
- Luigi Genovese (CEA) - WP3 leader
- Mariella Ippolito (CINECA) - WP7 Leader
- Luisa Neri (CNR) - WP10 Leader
- Marnick Bernx (EPFL)
- Stefano De Gironcoli (SISSA)
- Alberto Garcia (CSIC)
- Anton Kozhevnikov (ETHZ)

In the period covered by this report (M7-M46) has met regularly by teleconference.

- 27/05/2019 by teleconference
- 28/02/2020 by teleconference
- 08/04/2020 by teleconference
- 1/10/2020 and 8/10/2020 by teleconference
- 5/3/2021 by teleconference
- 31/05/2022 by teleconference

In these meeting several common topics were addressed, spanning from the position of the CoE in the ecosystem; a continuous assessment of WPs and codes progress; the monitoring of the financial situation; the two required extensions and the relevant actions to take with the Commission; the preparation and internal review of the meetings with the Commission (Midterm Review (RP1) on September 20-21/07/2020; the CoEs Fitness Check on April 21, 2021; to the collective designing of communication, dissemination, and training activities aimed at maximising the MaX impact.

The minutes of each General Assembly are available in the G-drive archive of the MaX CoE.

1.2 The Executive Committee

The **Executive Committee (ExC)** is the supervisory body for the execution of the Project, conceived as a board of 5-7 individuals covering different areas of expertise who should envisage and plan activities to put into action the Director and the GA guiding lines. Its composition changed during the project life, following the changes of the partner teams.

The ExC meetings were not intended to substitute dedicated regular WP meetings, which were usually decided bottom-up among two or more WPs to face the different phases of the CoE activity. They were complementary, possibly addressing subjects that go beyond a single WP (e.g. inter-WP

collaborations and tracking). The aims of the ExC meetings were to identify issues to be addressed by WPs, to monitor the overall coverage of the issues raised by the reviewers, and to define actions to be suggested to the GA for approval or to the WPs for further refinement. Furthermore, the EC duties were to implement the decisions taken by the GA, taking the decisions needed to support their implementation, coordinate the actions of the WPs towards common objectives, monitor the development of the activities and interactions with stakeholders, and analysing any difficulties or new opportunities in the CoE development and determining the necessary actions.

The Executive Committee was originally composed by Andrea Ferretti (CNR), Daniele Varsano (CNR), Daniel Wortmann (FZ Jülich), Giovanni Pizzi (EPFL), Zeila Zanolli (ICN2), Carlo Cavazzoni (CINECA), Stefano de Gironcoli (SISSA), and Luisa Neri (CNR, permanent invited member). In October 2020, after Zanolli and Cavazzoni left the consortium, Fabio Affinito (CINECA) and Alberto Garcia (ICMAB-CSIC) were added. Eventually, in March 2021, Mariella Ippolito (CINECA) entered the committee and Luisa Neri changed her role to full member. The ExC has been selected by the General Assembly upon the proposal of the Coordinator.

EXECUTIVE COMMITTEE

new entries from 1.10.2020 in yellow
new entries from 05.03.2021 in green

composition

Name	Affiliation	Role	Notes
Andrea Ferretti	CNR	Chair	
Daniele Varsano	CNR		
Daniel Wortmann	Juelich		
Giovanni Pizzi	EPFL		
Alberto Garcia	ICMAB - CSIC		replaced Zeila Zanolli from 1/10/2020
Fabio Affinito	CINECA		replaced Carlo Cavazzoni from 1/10/2020
Stefano De Gironcoli	SISSA		
Luisa Neri	CNR		changed role: from invited to member from 05/03/2021
Mariella Ippolito	CINECA		new entry from 05/03/2021

Fig 3. The history of changes in the composition of the Executive Committee.

List of the ExC meetings and principal issues:

- 27/11/2018. Kick-off programme and organisation: tentative agenda to be discussed with the Management and the PIs + definition of new project deadlines and discussion on the suggestions coming from the EC Officer and the experience gathered with MaX (first phase).
- 25/09/2019. Structure and the contents of the new MaX website + discussion on the feedback related to MaX "operational style" after almost one year of project life.

- 17/03/2020. Set of actions for the dissemination and communication of codes developments in the next months + open issues and work plan for codes: i) documentation on GPU-readiness; ii) Newsletter; iii) Message to Psi-k, iv) Webinars, v) Psi-k 2020 Conference booth.

- 17-18/09/2020. Analysis of the reviewers' comments after the M18 review (meeting to discuss some of the points raised by the reviewers: i) AiiDA and security; ii) analytics & machine learning; iii) definition of metrics, with particular emphasis on energy-aware measures, iv) Data-oriented activities; v) plans for software architecture & documentation, vi) WPs interaction; vii) formal interactions with other CoE/Projects.

- 01/03/2021. Topics: i) communications and measures to maximise MaX outcome and visibility; ii) actions towards the new EuroHPC supercomputers (pre-exa and possibly peta); iii) actions towards libraries and codes to be completed and made visible; iv) MaX seminars.

1.3 The Software Quality and Management Board

This board has actually been thought of as a specific working group to ensure the best quality in software engineering. It is led by the WP4 leader (C. Cavazzoni at the beginning, then F. Affinito, CINECA) and members from all the flagship codes. *The Board has been actually inglobated within the Executive Committee*, to avoid for the WP4 leaders and the other members an excessive workload. Topics of interests have been discussed there, via a dedicated Slack channel, and in restricted meetings. The group has cross-checked the advancement and quality of software engineering.

2 Final report on Operational management of the CoE

The daily management of the Centre of Excellence has been ensured by the MAX **Management Team**, composed of personnel from the Coordinator's node Cnr Nano. The management team supported the Coordinator in her role and in relationship with the Commission, and performed all the needed activities to fulfil the DoA previsions in terms of effective implementation of the work plan and the successful completion of MAX deliverables and milestones.

The team has been led by the WP10 leader and project manager, Luisa Neri, and included the Cnr staff: Maria Bartolacelli, MAX Technical Secretariat; Maddalena Scandola, press office; Maria Grazia Angelini and Paola Corezzola, administration; Maria Celeste Maschio, training support. The Management Team met weekly to discuss actions to be undertaken in order to respect deadlines, milestones, etc., with the MAX Director and Cnr PI, Elisa Molinari, the Cnr co-PI Andrea Ferretti, the Training manager Daniele Varsano, and Nicola Spallanzani.

As defined in the proposal, and described in detail in the previous deliverable D10.1, the management focused its activity on people, interaction, community, skills, and talents. Several

activities have been performed since the beginning of the project in 3 specific domains: 1. Governance, monitoring and quality; 2. Administrative, legal and financial management; 3. Knowledge and communication management.

According to these domains, we highlight the activities in:

1. **Governance, monitoring and quality**:

- organisation of the governing bodies meetings and activities; management of dates, agenda, minutes; technical set-up of telco meetings;
- overseeing of reporting deadlines and quality control. The Management team has set the schedule for the internal deadlines and reviews of
    - all deliverables (38 in the span covered by this deliverable)
    - Midterm Report (RP1) and review (July 2021)
    - Fitness Check (April 2021)
    - update of continuous reporting tool in the EU Funding and Tender's Portal
    - Final Report (RP2) and review (September-November 2021);
- KPIs managing and updating (see *section 3* below);
- supporting the WP8 leader in organising events, managing information and data about the training events, preparing reports and communication activities;
- informing the network on the Open Access rules and continuously ensure the compliance of acknowledged publications with the EU rules;

2. **Administrative, legal and financial management**:

- supporting the Coordinator in carrying out all administrative, legal, and financial duties and relevant commitments with the Commission; to draft and coordinate the interactions with the Commission for the Amendments (see below);
- collecting information within due deadlines from partners, and continuously assessing the overall financial situation;
- receiving payments from the Commission and transferring fundings to partners;
- ensuring the respect of the Grant Agreement and the Consortium Agreement terms and conditions;
- supervising the sustainability path and the drafting of the long-term evolution business plan; to check the MaX-related commercial activities of the partners.

3. **Knowledge and communication management**:

- ensuring an efficient internal communication strategy: planning and updating of a common repository platform to ensure that partners are informed, engaged, and conscious of common activities, requirements, deadlines. A G-drive intranet has been organized and main news have been continuously shared by emails to the whole network or to specific mailing lists;
- sharing of information within the network through formal and informal meetings, sharing of relevant papers and documents;
- strictly collaborating with the WP9 communication team in

  - ensuring the development and updating of the communication plan;
  - discussing new activities to develop;
  - quality control of content management;
  - social media management, website design and collaboration to continuous updating;
- (co)organising of events, e.g., webinars, participation to conferences; e.g. preparation of materials for thePsi-k Conference 2022 (booth, event, printed materials, newsletter, promotion);
- participation in FocusCoE meetings (esp. WPs on sustainability, industrial activities).

2.1 Amendments to the Grant Agreements

During the life of the Centre, two amendments of the Grant Agreement turned out to be necessary for a better development of tasks related to the dissemination and uptake of the project. In particular, the outburst of the Covid19 pandemic had undoubtedly reduced and slowed down the opportunities for communication, dissemination and uptake activities, and the necessity to disseminate in the best way possible the MaX results led to these requests. No additional financial fundings were requested for the extension-period support.

1. AMENDMENT AMD-824143-7: 6-month zero-cost extension.

This first extension was deemed necessary to accomplish all activities and the achievement of all deliverables and milestones with higher impact and has been especially relevant for activities oriented to dissemination, to increase industrial uptake and sustainability, to training and to enlarging community involvement (many of the activities have been delayed by the Covid-19 pandemic).

This resulted in a modification of the duration of the project specified in Article 3 of the Grant Agreement: the end was postponed from Dec. 1, 2018 to May 31, 2022, with a new duration of 42 months, and in the postponement of the following deliverables.

- D10.4 “Final business plan: exploitation and sustainability; uptake”;
- D6.3 “Report on the simulations performed and scientific outlook”;
- D6.4 “Report on the general challenges still to overcome to bridge the gap between pre-exascale and exascale simulations”;
- D7.3 “Third (final) report on the activity of the High-Level Support services (third year)”;
- D8.3 “Second report on Training and Education”;
- D9.4 “Impact Assessment Report, final version”;
- D10.5 “Final report on CoE governing bodies activity”;
- D10.6 “Final report on MAX in the European, national, international HPC ecosystems”.

2. AMENDMENT AMD-824143-20: 4-month zero-cost extension.

This further 4-month extension of the project duration has been especially relevant for activities oriented to dissemination, uptake and sustainability, training and community involvement, as well as for impact on the evolving European HPC ecosystem. In addition, it allowed us to avoid discontinuities in view of future projects that might result from forthcoming calls.

One specific reason for the request was to allow the Consortium to attend one of the events of main importance and impact for its community: the Psi-K conference, the major conference in the domain, scheduled every 5 years, and postponed to an in-person edition on August 22-25, 2022. MaX planned and implemented a dissemination event as a satellite to the conference, and other specific contributions to it. This has been a major showcase for MaX overall results and the dissemination legacy of the project. The conference registered over 1,250 participants. (See a detailed description in D9.4).

Furthermore, the request was justified by the necessity to synchronise with the EU-wide HPC ecosystem and machine deployment; as an example, while both LUMI and Leonardo pre-exascale machines had been meant to be deployed and become operational in Q4-2021, the development was still in progress at the stage.

The second amendment led to a postponement of the end of the project to month 46 (September 30th, 2022) and of deliverables:

- D10.4 “Final business plan: exploitation and sustainability; uptake”;
- D6.3 “Report on the simulations performed and scientific outlook”;
- D6.4 “Report on the general challenges still to overcome to bridge the gap between pre-exascale and exascale simulations”;
- D7.3 “Third (final) report on the activity of the High-Level Support services (third year)”;
- D8.3 “Second report on Training and Education”;
- D9.4 “Impact Assessment Report, final version”;
- D10.5 “Final report on CoE governing bodies activity”;
- D10.6 “Final report on MAX in the European, national, international HPC ecosystems”.

3 Key Performance Indicators (KPIs)

During the life of the project, MAX KPIs have been assessed regularly. The targets have been reached and exceeded in all areas, mirroring the continuous rich activity of the consortium. In the following a complete assessment of the KPIs is given.

In particular, the Software Development KPIs (related to actions addressed by WP1-3) provide a perspective on the advancements in the refactoring process of the MAX flagship codes: a large number of refactored code components are tracked at M46, 3 with *beta* and 25 with *production* readiness level (K1.1). At the same time, 23 new code functionalities (K3.1) and 14 algorithmic improvements (K3.2) - some of which were not possible before the pre-exa architectures - were implemented. Concerning performance portability (K2.1), the MAX flagship codes were tested and ported on up to 15 different architectures, resulting in an average of 8.4 architectures per code. Noticeably, all codes were ported on GPU-accelerated systems, some experience on AMD GPUs has

also been gathered, and ARM architectures were tested both with SVE or GPU acceleration (and also, importantly, on AWS Graviton3 chips).

Concerning the area of Exascale, Co-design and Data handling (related to the actions addressed by WP4-6), we report that beside the planned benchmarking campaigns (K4.1) MaX personnel were able to participate several extra campaigns and preliminary access programmes, which turned out to be extremely relevant for the development of the codes. Furthermore, WP4 tested novel programming models (K4.2) on more than 24 kernels of interest for the MaX community.

The advancements of Extreme Scale Pilot projects (K6.1) started at full speed after M12 as this KPI is largely tied to the availability of heterogeneous machines and ported MaX codes. By the end of MaX-phase 2, the result of 9 completed and 3 still-in-production demonstrators is a remarkable outcome.

The Services offered by MaX and handled by WP7 tracked over 2800 (1500+ from M18) support requests (K7.1), revealing a large activity of the MaX users and developers. Concerning training, almost 10.4k days of person-training have been delivered (~9k+ from M18) (K8.1). The sharp increase in the delivered training is due to the fact that most of the training since month 24 has been recast in an online format. The high quality of the proposed MaX training activities emerges from the user satisfaction rates, equal to 4.7/5 (K8.2).

About 100 scientific papers were published after M18 (K9.1), well beyond the target (25/year), all compliant with the OA policy. Another relevant aspect of MaX activities is given by the over 40 collaborative actions (K10.1) made by MaX members within the European HPC ecosystem.

Please note that all KPI targets for M36 have been translated to M46 due to the project's extension.

	#	Key Performance Indicator	KPI definition	target	M6	M12	M18	M24	M36	M46
Software Development	K1.1	Refactored code components	Number of software components (libraries, modules, building blocks) identified and refactored as self-standing objects	≥ 15						
			production		5	8	16	19	22	**25**
			beta		9	13	8	9	6	3
	K1.2	Impact of MaX libraries	Average (over libraries) number of codes (inside/outside MaX) using each MaX library	≥ 2	1.24	1.57	1.71	1.90	1.90	1.90
			used = 2		5	8	8	13	13	**13**
			used > 2		0	2	3	6	6	**6**
	K2.1	Portability on different architectures	Number of new ports of Max codes' components (eg KNL, intel+GPU, power+GPU, ARM) to different hardware architectures	≥ 2-3/component						
			# architecture addressed		3	10	10	11	12	**15**
			#average per code		2.5	5	6	7	7.4	**8.4**
	K2.2	Auto-tuning of code components	Number of intra-code components that have been tuned	≥ 4-5	4	6	7	7	7	**7**
	K2.3	Code exploitation of HPC machines	Number of MaX codes able to exploit in a single run a partition of a Tier0 machine which provides at least X% of the maximum available performance	7						
			#codes > 10%		5	6	7	7	7	**7**
			#codes > 20%		3	4	5	7	7	**7**
	K3.1	New code functionalities	Number of new physical functionalities enabled to run in a massively parallel environment	≥ 10	0	2	10	14	22	**23**
	K3.2	Algorithmic improvements	Number of code functionalities enabled by algorithmic developments from WP3	≥ 7	4	9	11	12	14	**14**

	#	Key Performance Indicator	KPI definition	target	M6	M12	M18	M24	M36	M46
Exascaling, Co-design & Data handling	K4.1	Profiling and benchmarking	Number of profiling and benchmarking campaigns	≥ 2/year	1	2	3	4	6	**8**
	K4.2	Programming models	Number of kernels tested with innovative programming models	10	4	9	18	20	23	**24**
	K5.1	Public workflows and turn-key solutions	Total number of workflows and turn-key solutions publicly released	≥ 12	53	70	79	89	108	**122**
			new workflows since M1		5	22	31	41	60	74
	K5.2	Quantum Mobile releases	Number of periodic releases of updated versions of the Quantum Mobile	≥ 2/year	3	7	11	12	15	**15**
	K5.3	Repository of materials data and workflows	Total number of validation runs (number of structures times number of codes), and of highly curated data present on the MaterialsCloud	≥ 50.000	0	15000	22000	40000	80000	**116000**
	K6.1	Tested Demonstrators	Number of Extreme Scale Pilot projects run and analysed	≥ 6						
			Test		-	3	4	2	2	0
			Production		-	1	3	6	3	3
			Complete		-	1	2	2	7	**9**
Infrastructure & Services	K7.1	High level domain-specific support	Total number of high-level support requests addressed by the CoE (trouble tickets, consultancy)	≥ 100/year	567	967	1278	1618	2296	**2861**
			helpdesk tickets		129	210	255	336	497	632
			forum/email threads		427	738	986	1232	1723	2132
			high level support actions		11	19	37	50	76	97
	K8.1	User uptake in MaX training events	Number of people trained in MaX training events (expressed in person days)	≥ 500/year	345	836	1530	1960	6752	**10428**
	K8.2	Training quality	Average evaluation assigned by participants in training events in anonymous questionnaires (values normalized between 1, negative and 5, optimum)	≥ 4.0	4.25	4.7	4.75	4.7	4.65	**4.7**
Dissemination, Exploitation & Management	K9.1	Dissemination	Total number of invited talks to conferences and schools (including event organization) + total number of scientific publications on international journals	≥ 25 papers/year + ≥ 75 invited talks/year	34 + 8	80 + 15	92 + 25	105 + 47	145 + 91	**178 + 128**
	K9.2	Communication and Outreach	Total number of people in the MaX network (social media followers, newsletter subscribers)	≥ 1000 followers by M12	1557	1723	1859	2183	2831	**3366**
	K10.1	Coordination with pan-European and national HPC ecosystems	Number of collaborative actions (eg participation to working/advisory groups, EuroHPC meetings, etc) to support the HPC ecosystem	≥ 8/year	9	29	43	52	70	**92**

4 Quality assessment & risk management

The Consortium considers **Risk management** an integral part of the project lifecycle, useful to minimise possible deviations from the expected results and schedule. Specific Risks and Contingency plans are defined for every WP and are presented and discussed in the DoA (*Section 1.3.5 WP5 Critical implementation risks and mitigation actions*). While at M18 a re-assessment of risks was performed, with two Covid-19 unforeseen risks added, at the end of the project we only perform an analysis of risks from the Risk Assessment Table, and discuss those that have incurred, including R4, R6, R7, R10, R12.

R1. The collection of code components identified and slated for encapsulation, optimisation, and reuse does not cover the full functionality of MAX codes. The software development plan was flexible enough to include the development of libraries that were not originally planned. One case is that of the DevXlib library, a performance portability tool developed directly within MAX to ease the adoption of multiple programming models for GPU support.

R2. Specific architecture our codes are tuned for, will come to an end of lifetime due to vendor decisions. Although some architectures (e.g., Intel KNL or IBM Power9) are not supposed to be further developed (and would go out-of-use in the short term, if not already), this risk was not critical as the work of MAX about portability was not tied to specific architectures and was carried out by constantly monitoring the evolution of the HPC hardware.

R3. The release of specifications of the planned pre-exascale machines and their deployment is delayed, and we will not be able to adjust our efforts accordingly. MaX has been working with HPC Centres in order to support all the available Tier-0 supercomputers in Europe. The deployment of pre-exascale machines has been delayed and they will be fully accessible only after the end of MAX phase 2. Nevertheless, we made contact with the consortia and had preliminary access to trial nodes of the relevant architectures (especially relevant in the case of LUMI). For instance, this ended up in the organisation of a MAX hackathon oriented to AMD hardware.

R5. In T4.1 the available implementations of programming models to be tested have a TRL too low for use with main trunk codes and full applications. MAX has carefully evaluated the evolution of most common programming models relevant to HPC (notably those aimed at supporting GPUs available for modern Fortran, tested them on software toy models, waiting for their adoption in the main branches of our codes by when they were ready. Moreover, the development of DevXlib has also been found crucial to hide part of the complexity of programming models in the scientific parts of the codes

R8. In T4.4 there is a risk of not having enough computational resources to properly run all benchmarks and profiling campaigns. The risk did not occur, as for the campaigns we leveraged not only the hours allocated by PRACE dedicated to CoEs, but we also exploited additional resources provided in-kind. Nevertheless, an increase in the budget allocated to the CoEs dedicated to

application development would be of great use for benchmarking and profiling, which is crucial for the success of CoEs' activity.

R9. In task 5.1, supercomputing centres could adopt new fast schedulers optimised for HTC on exascale machines that have a very different implementation logic from the existing ones and require significant changes to the AIIDA API. The risk did not occur as demonstrated by the HTC runs in Marconi 100 and more recently on the full LUMI-C partition as described in D5.7. Moreover, the use of meta-schedulers such as HyperQueue, already demonstrated on the LUMI-C runs using AiiDA, tends to further simplify the situation.

R11. In task 5.4, the data needs of the community might grow much faster than expected and the running costs of long-term storage exceed the current targets. The risk did not occur: The MaterialsCloud portal, by storing only curated data, demonstrated to be effective in short and medium term and we believe it is an adequate tool also for the long term.

R13. The viability of the realisation of these MAX Demonstrators relies on the availability of supercomputing resources. The risk did not occur, in some cases the needed resources were secured by applying to PRACE and national calls.

R14. **Difficulty to hire dedicated personnel for service provisioning in case of large custom development.** Personnel hiring, especially aimed at service provisioning and software development, turned out to be critical, nevertheless the mitigation measures conceived at M18 were successful and we did not experience delays in the project. In the future, we will leverage on separation of concerns (separate materials science and software engineer competence) to simplify the hiring process.

R15. The planned training offer is insufficient with respect to the requests. Having the greatest part of training been offered online in the last months, all applicants have always been accepted. All lectures were also recorded and made available for self-training in the MAX YouTube channel. A different case was the particularly successful event "*MAX school on Advanced Materials and Molecular Modelling with Quantum ESPRESSO",* which took place online on May 17-28, 2021: for organisational reasons only 120 participants were admitted to the school out of 1292 applications received. The entire school was video-recorded and is now available on the web for all interested students. Other editions of QE schools have been planned to widen the audience of attendees.

R16. There is limited interest in the education and training offered by the CoE and **R17 Users and stakeholders not responsive to the selected communication & dissemination channels.** The risk did not occur. All the contrary, as it is possible to see from KPIs (see above) that we had a great attendance in our events and abundantly overcame our targets concerning training.

R18-U1. Participation to pan-European, European, national initiatives in the HPC ecosystem and on policy and technical issues. As described in D10.6, partners attended a great number of events and maintained their position in the ecosystem, in spite of the pandemic.

U2. New COVID-19 (or similar) outbreak, with delays in spending, hiring, performing the due activities, reporting. The pandemic lasted longer than expected, with different degrees of severity

and limitations. The CoE activity never stopped, thanks to the unremitting work carried on by the partners. We intensified our online collaboration and pushed it forward, developing an extensive expertise in organising online activities and events, both for internal and external purposes, such as, e.g., dissemination and training.

U3. Partners are not able to hire the personnel needed to deliver some tasks. We dealt with the difficulties in hiring or starting new contracts due to the mobility restrictions when these were lifted, allowing new personnel to start their work. On the other hand, a major effort by staff helped the partners accomplish the planned tasks with no delays in the project.

No unforeseen risks arose during the period of this report.

5. Conclusions

The activity described in this deliverable was planned in WP10. It has been performed mainly by the management team, set in Cnr Nano in Modena. As MAX as a CoE had been established in 2015, the partners had already developed a long-term experience of collaboration, and the structure of management and governance had already been set. Nonetheless, the management team acquired a greater experience in this second phase, smoothed over, and profited from the consolidation of the CoE. This helped the network profitably go through the difficult years of the pandemic. Risks management and the topping of expected KPIs show the successful management and completion of the CoEs. WP10 worked jointly with all partners and WPs, though it had a tighter collaboration with WP8 and WP9, which helped in the development of plans, strategies, and tools, pushing the CoE to fulfil all its tasks.

The CoE governance has been able to respect its tasks and assignments and has fruitfully helped the Coordinator in her duties, and no issues need to be pointed out.

Activity within the Tasks *T10.3 Coordinating with pan-European and national HPC ecosystems* and *T10.4 Interfacing with international HPC materials research ecosystems* are described in D10.6 “Final report on MAX in the European, national, international HPC ecosystem” (M46), while D10.4 “Final business plan: exploitation and sustainability; uptake” (M46) describes the work done for *T10.5 Sustainability path and long term business plan*.

Appendix I. Risk Assessment Table (RAT) updated at M18 (RP1).

Risks are assessed as LOW, MEDIUM, HIGH.

RISK No.	DESCRIPTION OF THE RISK	M1	WP N.	PROPOSED RISK MITIGATION MEASURES	M18	MOTIVATION OF VARIATION AND CORRECTIVE ACTIONS FOR MITIGATION - M18
R1	The collection of code components identified and slated for encapsulation, optimisation, and reuse does not cover the full functionality of MaX codes.	MED	WP1	Target also code-specific modules for optimisation and interfacing work.	MED	Libraries that were initially unforeseen were included in the software development plan. One case is that of the DevXlib library, a tool for performance portability developed directly within MaX.
R2	Specific architecture our codes are tuned for, will come to an end of lifetime due to vendor decisions.	MED	WP2	Our work will not only focus on performance but also on portability to minimise the dependence on a single specific architecture. Together with the activities in WP4 we follow the developments pursued by hardware vendors to avoid this to happen.	LOW	We have carefully observed the evolution of HPC hardware and the related architectures.
R3	The release of specifications of the planned pre-exascale machines and their deployment is delayed, and we will not be able to adjust our efforts accordingly.	MED	WP2	Through our connections to PRACE-partners we will aim at using the most advanced European supercomputers available Furthermore our focus on performance portability should also allow us to produce codes easily adjustable on the final pre-exascale machines.	HIGH	No significant delays in the deployment of pre-exascale and exascale machines has been observed. If any, the release of OneAPI and OpenMP5 implementations has been postponed several times. Indeed, we have worked with HPC Centres in order to support all the available Tier-0 supercomputers in Europe. For instance, we have been working both on GPU-accelerated as well as on non-accelerated ARM architectures. Moreover, our

						approach to performance portability has been designed and developed in such a way to be as HW agnostic as possible.
R4	Code components identified in WP1 take longer to be extracted.	MED	WP3	Focus the initial developments to the implementations that require less restructuring of the host application. Provide immediate feedback to WP1 work-groups should a design problem in the application components arise.	MED	The risk did not occur. In a few cases the completion of code component extraction has been postponed, but the main reason is rescheduling (eg, in favour of the development of performance portability tools) rather than design or unexpected problems.
R5	In T4.1 the available implementations of programming models to be tested have a TRL too low for use with main trunk codes and full applications.	MED	WP4	Use mini-apps or relevant kernels to validate the paradigm, before considering the full application. Consider different implementations (e.g. at least two compiler technologies), preserve fallback solutions if appropriate.	HIGH	The risk occurred and the description adapts very well to the case of OpenMP5 and Intel OneAPI (to be used e.g. with Intel "Ponte Vecchio" GPUs, or AMD GPUs). The AMD tool chain (ROCm) has also experienced some delays in being delivered (e.g. missing linear algebra tools).
R6	In T4.2 there is a risk of not being able to assess memory usage and then not being able to find solutions to exploit new memory for exascale systems (low risk).	LOW	WP4	In all the assessment and co-design tasks we will consider at least two MAX flagship codes.Well established profiling tools will be used and we will ask for consultancy to experts from FET projects dealing with memory technology and other CoEs (e.g. POP or SAGE2), as already occurred in the first implementation of MAX.	LOW	The risk did not occur.
R7	In T4.3 there is a risk of not being able to properly feed the co-design cycle.	LOW	WP4	Consult experts in co-design coming from architecture specialists (Arm and external contacts) and integration companies (E4) as well as involve code developers. We will consider many co-design vehicles and codes, so we have a high probability of having enough code base	LOW	The co-design activity developed well and the risk did not materialise.

				and test cases to keep the co-design cycle alive.		
R8	In T4.4 there is a risk of not having enough computational resources to properly run all benchmarks and profiling campaigns.	LOW	WP4	Define at least one benchmark with large code coverage for each application that will be prioritised. We will calibrate the input dataset and limit benchmark run to few iterations, in order to fit in the in-kind resources available through HPC centres (e.g. CINECA commit to deliver 50K node/hours each year to run benchmarks at scale). Moreover,the benchmark team will apply for CPU grants at national and EU level (e.g. through PRACE preparatory program).	MED	So far we were able to run benchmarks by using the CoE-dedicated resources of PRACE and additional resources that we have provided in-kind. For instance, CINECA has granted a 2 week pre-production access to a number of MaX developers to perform benchmarking on the newly deployed Marconi100 machine. Nevertheless, the issue of accessing computational resources for software development and benchmarking is still there and a quite critical one. We strongly advise for a significant increase of the PRACE budget for CoEs and/or for development in general. Note also that the programs accepting development, validation, and verification work as the main goal of the proposals are quite limited or absent, while these activities are crucial for the development of a healthy software ecosystem.
R9	In task 5.1, supercomputing centres could adopt new fast schedulers optimised for HTC on exascale machines that have a very different implementation logic from the existing ones and require significant changes to the AIIDA API.	LOW	WP5	periodic interactions of AIIDA developers with supercomputer centres to know well in advance novel scheduler models and have time to adapt the API.	LOW	No occurrence (e.g. most PRACE Tier0 machines based on the SLURM scheduler, well supported by AiiDA). Indeed, we were able to perform large scale high-throughput calculations on the recently deployed Marconi100 machine (IBM P9 + Nvidia V100 GPUs) during the very early days of the machine.
R10	In task 5.2, some codes could be difficult to fully automate or might have high non-convergence or failure rates.	MED	WP5	Minimise impact: provide turn-key solutions that give the user more input options when their choice is hard to automate, document their meaning; implement	LOW	While non-convergence rates or difficulties in automation exist (these are the problems developers have to face on a daily basis), no unforeseen or critical behaviours have been found. All

				workflows to recover from failed runs. Continuous iterations between high-throughput researchers and code developers to highlight critical cases, giving developers detailed problematic cases and enough time to make the codes more robust.		developments in this context have followed the plans.
R11	In task 5.4, the data needs of the community might grow much faster than expected and the running costs of long-term storage exceed the current targets.	MED	WP5	Implement per-user/per-project quotas to ensure sustainable limits. Monitor size growth of submissions to act on time in order to minimise risk impact.	LOW	The risk did not materialise. One of the reasons is also the design of the MaterialsCloud portal. Within this initiative we focus on curated data (at variance of automatic dumping/storage of all data and all calculations). While avoiding technical issues, we also consider this strategy the most effective in the short, medium, and long terms.
R12	In task 5.6 pilot 1, the amount of data might not be enough to train a reliable neural network for performance prediction.	LOW	WP5	Complement the neural-network predictions with performance models based on code flow analysis, using hardware performance information as input. Act early to implement automated processes to collect data statistics of runs.	LOW	The neural network approach of T5.6 pilot 1 has been numerically demonstrated as feasible (and the description of the approach was published in a scientific paper). Extension of the approach to more use cases (more codes, more kernels) is undergoing.
R13	The viability of the realisation of these MAX Demonstrators relies on the availability of supercomputing resources.	LOW	WP6	We have provisioned access to adequate resources via: –The integration of supercomputing centres in the MaX consortium. The team of each MAX flagship code is closely linked to a supercomputing centre participating in MaX (Quantum ESPRESSO and YAMBO with CINECA; SIESTA with BSC; FLEUR with Juelich; BIGDFT with CEA; CP2K with CSCS). These centres routinely provide computational resources for development, benchmarking	LOW	The strategies described in the "risk mitigation" have been put in place since the beginning of the MaX second phase. In particular we have applied for PRACE and National resources targeted to MaX demonstrators (both testing and production). Moreover, as described above in R8, we have organised, together with CINECA, a MaX-wide pre-production access to the Tier-0 machine Marconi 100, that allowed for large scale simulations on a GPU-accelerated machine.

				and debugging, and also large amounts of CPU time during the testing periods of newly installed supercomputers.–Access to PRACE resources, through their continuous calls for Preparatory Access projects.–As a backup plan, CINECA has committed to provide the computational resources needed to perform the activities in MaX Demonstrators (see Letters of commitment in Sec. B.6)		
R14	Difficulty to hire dedicated personnel for service provisioning in case of large custom development.	MED	WP7	A number of actions aimed at the training of SW developers has been identified and put in place in MaX WP8. This should provide a larger base of developers thereby minimising the risk.	MED	Personnel hiring, especially aimed at service provisioning and software development turned out to be critical. On one side we have exploited the critical mass of the MaX CoE by making a hiring network among the partners and exchanging information and candidate contacts. This turned out to be an effective strategy in a number of cases. Nevertheless, in some other cases we were not able to hire personnel in due time (especially SW developers with materials science competence). We foresee three possible lines of actions: (1) the separation of concerns, modularization, encapsulation ongoing and more and more in place in MaX codes will reduce the need of personnel with software engineering and materials science competence at the same time, hopefully easing hiring. (2) At the global level, policy actions are required to increase attractivity of such positions: e.g. by fostering visibility and career opportunities for people active in the development of scientific software, especially within the European HPC scenario. (3) We

						could try to involve more existing personnel of the partner institutions (typically researchers, but also PhD students). This has already happened in practice, but cannot be considered a viable strategy in general. As an extreme solution, we may agree with the involved partners that some activities may be taken over by a different partner.
R15	The planned training offer is insufficient with respect to the requests.	MED	WP8	Apply for additional support from other sources in order to increase the domain-specific offer, further coordination with PRACE and CSA to address requests. Training materials available online.	MED	In a couple of cases, MaX training events were strongly oversubscribed (e.g. the 2020 Yambo school at ICTP with more than 270 applications for 50 seats). On one side we have slightly extended the acceptance to 55-60 people, then we have recorded the lectures and provided all the training material online. In general this has been identified as a good practice for the MaX training, even more so with the outbreak of the COVID19 pandemics.
R16	There is limited interest in the education and training offered by the CoE.	LOW	WP8	Focused actions in event advertising in collaboration with WP9.	LOW	MaX training events have often been oversubscribed, so the risk did not materialise.
R17	Users and stakeholders not responsive to the selected communication & dissemination channels.	MED	WP9	Multiple different media and communication & dissemination strategies will be used, making the action flexible.	LOW	The risk did not occur. Events organised and participated, along with the different communication channels used for MaX touched an audience of about 50k people.
R18* U1	Participation to pan-European, European, national initiatives in the HPC ecosystem and on policy and technical issues.	LOW	WP10	Increase effort in sharing expertise by participating in working groups, organisingyui and attending events.	LOW	MaX members are active in several European institutions, networks. Strong ties have been established with Focus Coe and other CoEs and all the main institutions in Europe (EPI, PRACE, etc).
U2	New COVID-19 (or similar) outbreak, with delays in spending, hiring, performing the due activities, reporting.		WP1-WP10	Actions will be undertaken to keep activities going on as done during the first COVID-19 outbreak. While virtual meetings, virtual	HIGH	All members have been affected by the COVID-19 outbreak, and faced some setback in their work due to e.g. less powerful workstation at home; impossibility to meet and

				training events can be organised, and work from home can be pushed in order to reach the goals, an outbreak may affect the pace of activities and difficulties with spending and hiring, or person/effort in general, may arise. These need to be assessed within the consortium in the full respect of national restrictions and laws.		travel (our internal meeting planned for February 24-25 was promptly turned into a virtual one); need to cancel or reorganise and reschedule training or dissemination events; difficulty in hiring new staff, having full time work accomplished, etc. Unfortunately, the future perspective is not yet clear: we may have to face new delays and restrictions, and will need to rely again on the resilience and creativity of the whole consortium to cope with them (including possible reallocation of tasks).
U3	Partners are not able to hire the personnel needed to deliver some tasks.		WP1 -10	Besides all possible support given to complete hiring and deliver in time, reallocation of tasks to partners with available effort will be considered.	MED	