D9.2

Impact Assessment Report, mid-term version

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Due date of deliverable: 31/05/2020
Actual submission date: 04/06/2020
Final version: 01/06/2020

Lead beneficiary: Trust-IT (participant number 14)
Dissemination level: PU - Public

Document information

Project acronym:	MaX
Project full title:	Materials Design at the Exascale
Research Action Project type:	European Centre of Excellence in materials modelling, simulations and design
EC Grant agreement no.:	824143
Project starting / end date:	01/12/2018 (month 1) / 30/11/2021 (month 36)
Website:	www.max-centre.eu
Deliverable No.:	D9.2

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To be cited as: Muscella et al., (2020): Impact Assessment Report, mid-term version. Deliverable D9.2 of the H2020 project MaX (final version as of 03/06/2020). EC grant agreement no: 824143, Trust-IT, Pisa, Italy.

Disclaimer:

Versioning and contribution history

Version	Date	Author	Notes
0.1	17.02.2020	Julie Abergas-Arteza (Trust- IT)	1st first version Table of Contents (ToC)
0.2	03.03.2020	Stephanie Parker	Final D9.2 ToC
0.3	05.03.2019	Julie Abergas-Arteza (Trust-IT)	Request for MaX flagship codes contribution
0.4	03.04.2020	Stephanie Parker, Julie Abergas-Arteza (Trust- IT)	Send for WPs contribution
0.5	08.04.2020	Stephanie Parker, Julie Abergas-Arteza (Trust- IT)	1st round of inputs from Trust-IT, technical WP and task leaders
0.6	22.04.2020	Stephanie Parker, Julie Abergas-Arteza (Trust-IT)	2nd round of inputs by Trust-IT, technical WP and task leaders.
0.7	30.04.2020	Stephanie Parker, Julie Abergas-Arteza, Francesco Osimanti (Trust- IT)	3rd integration by Trust-IT and status report to coordinator and partners.
0.8	06.05.2020	Stephanie Parker, Julie Abergas-Arteza (Trust- IT)	Updates and edits
0.9	18.05.2020	Silvana Muscella, Stephanie Parker, Julie Arteza (Trust-IT)	Updated section 4
0.10	27.05.2020	Luisa Neri, Maria Celeste Maschio (CNR)	Revision of section 3 and overall edits

0.11	30.05.2020	Luisa Neri, Maria Celeste Maschio, Maria Bartolacelli (CNR)	New content added on impact assessment. Internal review and final edits.
0.12	03.06.2020	Silvana Muscella, Francesco Osimanti, Stephanie Parker, Julie Arteza (Trust-IT)	Final proofread check.

Content

Executive summary

This Report presents an assessment of the impact of the main outcomes of the MaX Centre of Excellence in its first 18 months. MaX is now established as a cornerstone of the European HPC applications ecosystem, and is recognized as a reference point in the computational materials research community.

MaX flagship applications and the workflow and data platforms have extended their global users pool, enabling them to take advantage of the forthcoming EuroHPC architectures for extreme performance and high throughput computing. The number of citations that the codes have received in scientific publication exceeds 4200 publications in the period January 2019 - May 2020 (over 10000 estimated single downloads/year). The number of participants who were directly exposed to MaX training activities in the same period exceeds 1000.

The report demonstrates how MaX activities impact all its stakeholders in industry and academia. This impact was supported by a massive effort on services and on networking, dissemination and communication activities. The consortium has also had to introduce an agile and results-oriented approach towards substituting scheduled, physical events due to the global pandemic to other means of virtual formats to help demonstrate the impacts of MAX.

The report also shows how strong relationships in Europe between main initiatives are brought to the table, including effective networking and collaborations within the EuroHPC Joint Undertaking and the EOSC community, with other HPC Centres of Excellence and all the actors of the European HPC ecosystem. It also shows the strong network of MaX with many domain specific initiatives such as e.g. the Psi-k, Cecam and the Graphene flagship project.

This Impact Assessment Report is submitted in the concluding year of Horizon 2020 whilst looking at distinct priorities for Horizon Europe, namely: Digital Transformation, Green Transition and Security & Autonomy[1], which are already at the core of MAX and will be key priorities in its work plan for the following years as well.

[1] https://ec.europa.eu/commission/presscorner/detail/en/ip_20_416 "Making Europe's businesses future-ready: A new Industrial Strategy for a globally competitive, green and digital Europe

1. Introduction

This report tracks the impact assessment of the MAX project in the period up to May 2020 (M18). Its focus lies in reporting on the latest MAX advances and engagement with all stakeholders under WP9. This WP, with WP8, is responsible for impacts related to skills development, dissemination and exploitation, including KPIs to measure tangible impacts in the EU HPC context and beyond.

D9.2 is part of an all-partner drive to maximize impacts and boost collaboration and uptake of HPC for materials science. Partner contributions include joint collaborative efforts with peer projects and the FocusCoE CSA, with which MAX has established a working relationship.

MAX will enable the successful deployment and ambitious evolution of the most widely used open-source, materials science community codes on pre-exascale machines by the end of the project in November 2021, and prepare them for the transition to exascale. MAX will also enable high-throughput computing, with a large number of simulations on pre-exascale machines, will provide HPC- and HTC-enabled software and concepts to the broad community of code developers, will support the convergence with high-performance data analytics and will foster the creation of a broad and skilled talent pool in Europe. Its ultimate goal is to boost the research based on HPC and HTC in industry and academia in the materials science and the related domains, and to contribute to the frontiers of the European and digital ecosystem.

The first part of this document overviews the impact of the impact of the activities deployed in the technical WPs of MaX. The second part is specifically centred on the communication and dissemination efforts deployed in WP9. More specifically, the rest of this document is structured as follows:

Section 2: Covers the strategy for impact assessment for stakeholder engagement, synergies and communication.
Section 3: Focuses on the overall impacts of MAX, spanning innovations, MAX tools and flagship codes.
Section 4: Reports on the impacts of stakeholder engagement through events, from training to webinars and 3rd-party events. It includes an overview of stakeholder views and a summary of impacts per stakeholder group.
Section 5: Details the impacts of the communication strategy, spanning the MAX website and engagement channels. It reports on overall impact assessment, including a dedicated dashboard and the KPIs, with an analysis of the community developed so far. Besides, some final considerations on how MaX benchmarked itself among the broad European and International HPC community.
Annex I: Contains the glossary of acronyms.
Annex II: List of Publications by MaX participants.
Annex III: List of MaX organised and participated 3rd-party events.

2. Strategy for Impact Assessments of the Communication and Engagement Activities

In D9.1 "MAX Communication and Dissemination Strategy & Stakeholder Engagement Plan" (M6) we outlined the plan for the project's communications, defined on the different stakeholders relevant to MAX. Below, we give a summary of the main goals and objectives for this strategy and analyze our

actions and their impacts up to M18.

Strategy for Stakeholder Engagement

- Profiling the MAX community in terms of the stakeholder groups, tracking community development impacts, including participants to webinars and other events (see D9.1). This includes periodical reviews of the groups in the MAX context.
- Identifying the most relevant venues for stakeholder engagement, such as 3rd-party events, as well as hosting MAX webinars and workshops.
- Promoting event participation, roles and networking opportunities for physical events.
- Reporting on event outcomes, takeaways and impacts. This includes outcomes of the interactive features of the events, such as the Q&A and the poll results, as well as the data collected in terms of geographical coverage and stakeholder categories.
- Ensuring regular community interactions through professional networks like LinkedIn and social media channels like Twitter.
- Measuring overall impacts of engagement, including training.

Specific groups of stakeholders need further approach, as, e.g, Institutional stakeholders, policy makers in the European and HPC ecosystem. Further actions for them, aimed at improving the existing synergies, are:

- Ensuring a coordinated and collaborative approach to HPC in Europe.
- Extending the MAX community of users, such as developers and users of the flagship codes and industry.
- Sharing insights and impacts across the EU cloud and HPC landscapes.
- Co-defining training requirements across diverse domains and target audiences, also in the context of European national programmes.
- Highlighting complementary results and impacts to policymakers.

Engagement with women in technology and science deserves a special mention. Steps to address current gaps in gender imbalance are aligned with the approach taken in WP8 and include:

- Tapping into networks of young women to increase engagement and women professors as potential role models.
- Tracking the number of women members of the MAX community and participating in webinars and workshops.
- Monitoring MAX participation in sessions on women in science and technology and initiatives within the project aimed at supporting greater participation.
- Making a careful selection of applicants for fellowships with a view to maximizing participation under WP8.
- Increasing the number of women involved in event organization, webinar panellists and roles in events in general (e.g. chairs, presenters, trainees etc.)

Strategy for communication

- Implementing the communication strategy defined in D9.1 (MAX Communication and Dissemination Strategy and Stakeholder Engagement Plan), which defines a set of KPIs against which impacts are monitored.
- Adapting the plan as necessary to reflect project developments and in the face of situations such as the COVID-19 pandemic with event cancellations and postponements.
- Intensifying other forms of engagement, such as webinars, videos, newsletters to ensure the

community keeps abreast of developments and new opportunities, working closely with the synergies established.

- Carrying out large-scale promotional campaigns for the webinars across the MAX network and relevant synergies.
- Populating the MAX website and measuring impacts automatically generated through a dedicated dashboard.
- Carrying out weekly campaigns on Twitter and LinkedIn, including SMART-based campaigns for events, with a clear start and end date and measurable targets.
- Measuring overall impacts of the communications strategy.

2.1 Engagement Levers

To achieve its strategy for communications and stakeholder engagement, MAX implements a set of practical levers, as depicted in the image below.

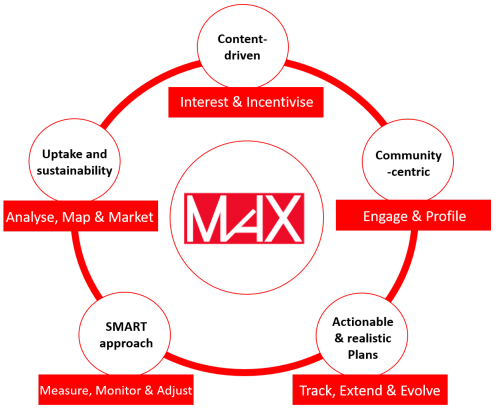


Figure 1: MAX *levers for stakeholder engagement*

In practice, this entails:

- **A content-driven approach**: tailoring MAX and external content in a way that interests the community of stakeholders with clear calls for action to engage with the project and its communication and dissemination activities.

- **Community-centric**: focusing on the information needs of the diverse stakeholder groups targeted by MAX, such as incentivizing the developer community; showing the benefits of using the flagship codes; understanding the advantages for industrial users not just to out-compute but to out-compete; showcasing results to policymakers across the EU.

- **Actionable and realistic plans**: regular planning updates that reflect the status of the project's outputs across its technical developments. This entails tracking, extending and evolving as the project matures over time and increases its readiness levels for uptake.

- **SMART approach**: creating promotional campaigns that have a clear start and end date, that are targeted to specific audiences and can be measured, monitored and adjusted as necessary.

- **Uptake and sustainability**: positioning MAX in the HPC for materials science ecosystem with clearly defined value propositions, analyzing uptake potential and leads within the community database for targeted actions; mapping assets with stakeholder groups and marketing the assets based on real opportunities. The impacts of MAX are critical for boosting uptake and sustainability beyond the funding life-cycle.

Brand recognition comes from combining these elements with the MAX value proposition as a Centre of Excellence within the EU. Diverse formats and mechanisms are used to engage stakeholders with tailored content and updated over time, including a set of training presentations and tutorials clustered by stakeholders and topics. These are published and used at various MAX events, training sessions, workshops, and 3rd party events, and are available for re-use as the community expands.

3 Overall MAX Impacts

The main goals for MAX impacts, as established in the project, include:

- European leadership in exascale and extreme-scale -oriented codes and innovative algorithms and/or solutions that address societal challenges or are important for key scientific and industrial applications in the materials domain;
- Improved access to computing applications and expertise that enables researchers and industry to be more productive, leading to scientific excellence and economic and social benefit; improved competitiveness for European companies and SMEs through access to CoE expertise and services;
- Federating capabilities and integrating communities around computational science in Europe;
- A large number of scientists and engineers, in particular female and young ones, trained in the use of computational methods and optimisation of applications.

As set out in the project, several measures have been planned in order to disseminate and exploit the results of MAX and to engage as much as possible the relevant communities. This is done by: broadcasting of MAX results as broadly as possible across the European HPC ecosystem and beyond; a concerted approach to HPC skills development through an extensive training programme; a coordinated and collaborative approach in the EuroHPC context.

The MAX flagship codes, with their improved capabilities and their evolution towards (pre-)exascale architectures, together with the MAX information and data platform, are the main outcome of our activities, and their impact involves all categories of stakeholders. We thus discuss them specifically in the next two sections 3.1 and 3.2. In section 3.3. we briefly report on MAX services supporting the uptake of MAX codes, also relevant to all stakeholders. Finally, in section 3.4 we review the impact of MAX activities according to the main categories of stakeholders. The discussion of specific communication and dissemination action is left to the subsequent Sections.

3.1 Flagship codes impact

As a result of the work carried out from WP1 through to WP4, the MAX flagship codes (Quantum ESPRESSO, SIESTA, cp2k, YAMBO, BigDft, FLEUR) are now able to run on the pre-exascale hardware with good performance, and are being prepared for the expected exascale evolution of architectures. Codes have been strongly refactored and modularised (separation of concerns, encapsulation), components start to be exchanged among them and become available to other codes. At the same time, MAX codes continue to evolve rapidly with new capabilities (e.g. calculated materials properties and algorithms). Importantly, all MAX codes are now ready for efficient high-throughput use, thanks to the information and data platform (AiiDA and Materials Cloud) developed in WP5. All codes and high-throughput tools developed within MAX are used in production for scientific publication, and through registering data in FAIR compliant repositories. More about these advancements is reported in the technical deliverables.

This huge effort has allowed to strengthen the use and impact of MAX codes in the European and global landscape. As indicators of the impact of MAX flagship codes, we report:

- the number of code downloads, estimated to **> 10000 single downloads/year**, and the number of citations that the codes have received in scientific publications: it is **over 4200 publications in the period January 2019 - May 2020**, according to ISI citation index (out of which 2766 for Quantum ESPRESSO, 945 for Siesta, 448 for CP2K). A total 66 additional citations refer to the AiiDA platform.
  The impact in different geographical regions is given in the first map, reporting the number of papers quoting the MAX flagship codes with a given European country in the affiliation. In the case of multiple authors from the same countries, the publication is counted once for each country. For reference, the second map shows the corresponding results at a global level. It is very easy to see the wide usage of MAX's codes all over Europe and globally.

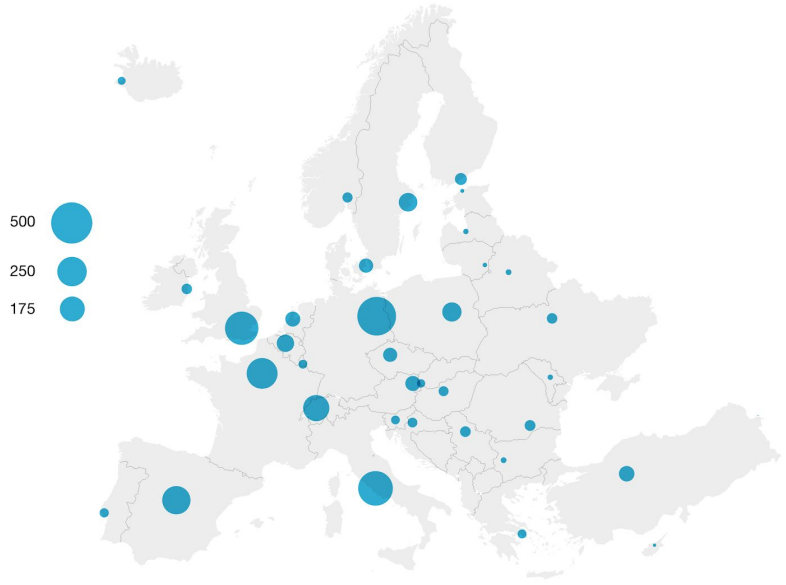


Figure 2. Geographic distribution in Europe of author affiliation in papers citing the flagship codes.

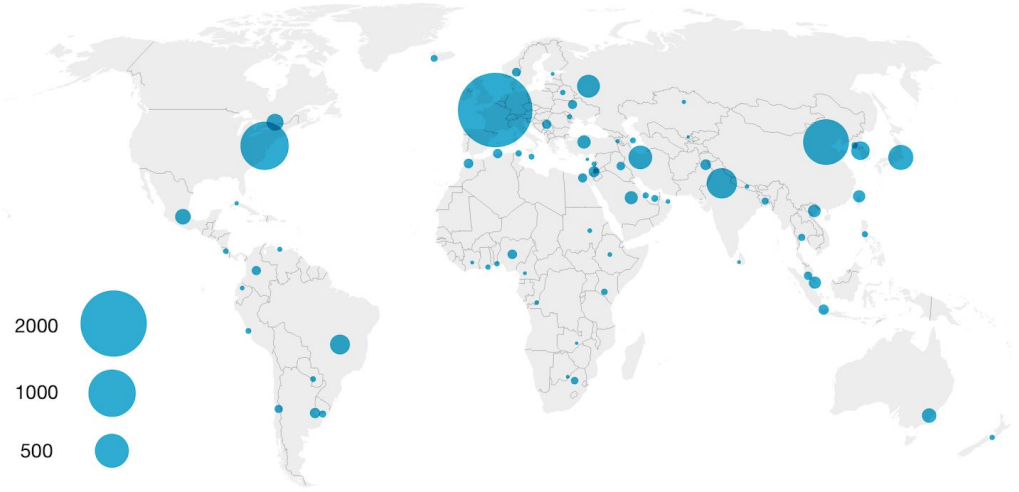


Figure 3. Geographic distribution all over the world of author affiliation in papers citing the flagship codes.

- the number of community developers: we count **over 100 active developers** involved across all the MAX flagship codes;
- the number of **PRACE projects using MAX codes**. An analysis performed on the "Chem. sci. and materials" domain of PRACE for the electronic structure codes subset shows that the number of projects using a MAX flagship code is **52% of the total** (was 50% in May 2017), and **over 89% of those using open source codes**. In particular in PRACE calls 18-19, **16 projects** are based on Quantum ESPRESSO, **6 projects** on Yambo, and **1 project** on CP2K. More details on the data are reported in D10.3.

The uptake of MAX flagship codes was supported and witnessed by a large number of diverse training activities, which involved directly **over 1000 participants** (more details about the individual activities and their evaluation are in deliverable D8.2):

- events that took place before COVID-19 outbreak:
  - organization of 3 schools with hands-on sessions dedicated to the flagship codes, involving **125** students;
  - organization of 5 Hackathons and workshops aimed at training code developers, involving **142** participants;
  - participation in schools organized by other institutions (total of 11 MAX expert members participated as trainers) (more than **310** students);
  - contributions to **4** Master programmes with introductory courses on computational materials science, hands-on sessions on usage of MAX flagship codes and best practice in their usage in HPC facilities
  - **38** researchers hosted at MAX laboratories for basic and specialized training on MAX codes and libraries
- a series of webinars presenting to the scientific and industrial community the advancements in codes including the porting to heterogeneous architectures. So far, two out of them took

place while two are already planned and advertised and are available in the MAX website for future reference. They were attended by about **320 active participants** from different stakeholder groups.

- Webinar: How to use Quantum ESPRESSO on new GPU based HPC systems. April 23, 2020.[2]
- Webinar: Managing, simplifying and disseminating High-Throughput computational materials science with AiiDA, AiiDA lab, and the Materials Cloud Archive. May 27, 2020.[3]

All the other communication tools also contributed to support the impact of MAX codes: newsletter, website, social media. Details are given in Section 5.1 below.

Figure 4. Announcing the MaX Flagship codes webinars.

3.2 Automated workflow and data platform impact

MAX enables the evolution towards exascale computation also by supporting high-throughput automated workflows through Aiida.

A measure of its impact and community engagement is the number of supported codes: it is steadily increasing, now over 45 packages and over 80 code executables are supported. Among them, all MAX codes are of course included. The list of the plugin packages in the Aiida registry (https://aiidateam.github.io/aiida-registry/) show:

- Calculations: 89 plugins in 35 packages
- Parsers: 79 plugins in 35 packages
- Data: 61 plugins in 21 packages
- Workflows: 80 plugins in 17 packages
- Others: 114 plugins in 22 packages.

Concerning the data and information ecosystem, MAX develops Materials Cloud, a web portal to foster Open Science, in collaboration with MARVEL and other community projects. Materials Cloud is constantly growing in terms of users and curated data. Table 1 collects selected Materials Cloud statistics.

[2] http://www.max-centre.eu/webinar/how-use-quantum-espresso-new-gpu-based-hpc-systems
[3] http://www.max-centre.eu/webinar/managing-simplifying-and-disseminating-high-throughput-computational-materials-science-aiida

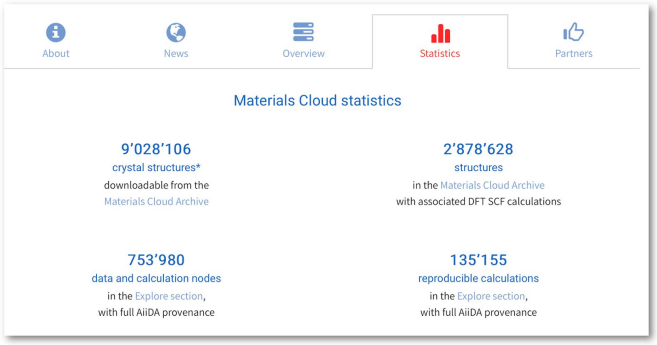


Table 1. Selected Materials Cloud statistics (December 2019).

3.3 MaX services impact

The focus of MaX services is on domain-specific user support and on consulting to users of HPC electronic structure codes (MaX codes and beyond). The effort deployed by WP5 has been essential to allow the broad users impact discussed in the previous sections. Importantly, all activities resulted from the synergic effort of the help desk supported by HPC centres (especially Cineca), by the code developing teams through the dedicated forum and mailing lists, together by all MaX partners for high level support actions. A detailed report for the first year of MaX is available in D7.1. Here we just emphasize the following facts and figures:

- **210** helpdesk tickets (out of which 112 for non-MaX codes)
- **740** incoming threads (code forum or mailing list)
- **1070** gitlab threads
- **2270** emails/posts
- **30** face to face support actions
- **20** high level support actions

The best confirmation of the success of these activities is in the strengthened use of MaX codes described in the previous paragraphs.

3.4 Impact towards priority stakeholders group

In the effort of maximizing impact, several groups of stakeholders were identified in the project as those who may take the greatest advantage from MaX's results and actions towards them described in the communication and dissemination plan .

In the following we give an overview of MaX activities towards those stakeholders and assess the impact we have produced so far. It must be stated that activities are not sharply cut but can of course involve several different groups at the same time, as they often overlap.

The paragraphs below report the major actions taken for the four main MaX stakeholder groups: i) European institutions and ecosystem; ii) industry; iii) research and academic institutions; iv) the general public.

3.4.1 European institutions and ecosystem

A very extensive description of the activities with these stakeholders is given in the D10.3 ("First report on MaX in the European, national, international HPC ecosystems"), so here we mention them briefly and refer to that deliverable for full information.

MaX has long-term ongoing synergies with the key players of the European HPC ecosystem such as EuroHPC Joint Undertaking[4], PRACE[5], EPI[6], ETP4HPC[7], EOSC[8], CoEs and FocusCoE[9], and with major players of the materials research ecosystem, including Psi-k[10], and CECAM[11], Graphene Flagship[12] among others, to capitalize on established networks and carry out joint dissemination towards scientific, research, industrial stakeholders and HPC-related projects and initiatives. A summary of the institutions involved in MaX networking actions is shown in Fig. 5.

Synergies have primarily developed on the technical plan: MaX has been extremely successful in coordinating and establishing collaborative actions with the key players of the European HPC. To remind just one example, MaX has been collaborating with EPI systematically on common co-design initiatives, communicating findings about MaX codes and co-design vehicles (mini-apps, libraries).

On a policy-making plan, MaX experience is being exploited and mirrored in these organizations' activities as many MaX participants have a role in their boards, such as E. Molinari (coordinator) and C. Cavazzoni (WP4 leader) are members of the EuroHPC Research and Innovation Advisory Group (RIAG) and have contributed to the Strategic Research and Innovation Agenda 2019[13] and to the Multiannual Strategic Research and Innovation Agenda 2021/2022; E. Molinari is Vice Chair of the HPC CoE Council - HPC3 of Focus CoE and several other MaX participants are members of its working groups; S. Muscella (WP9 leader) is the EOSC High Level Expert Role Group chair; C. Cavazzoni is member of the ETP4HPC Steering Board; N. Marzari (WP5 leader) is chair of the Psi-K Board of Trustees and E. Molinari is a member.

MaX members have participated in several events organized by European institutions (some of them were jointly organized), contributing with their knowledge and experience. Among others:

- EuroHPC Policy + Digital Excellence Forum (Helsinki, 19/09/2019)
- Graphene Flagship – MaX joint workshop on "High-performance computing for 2D materials research" (Helsinki, 24/09/2019)
- EOSC-hub week: "Pathways for EOSC-hub and MaX collaboration. A platform for reproducible science with full provenance" (G. Pizzi) (Prague, 10-12/04/2019)

[4] https://eurohpc-ju.europa.eu/.
[5] https://prace-ri.eu/.
[6] https://www.european-processor-initiative.eu/.
[7] https://www.etp4hpc.eu/.
[8] https://www.eoscsecretariat.eu/node.
[9] https://www.focus-coe.eu/.
[10] https://psi-k.net/
[11] https://www.cecam.org/
[12] http://graphene-flagship.eu/
[13] https://eurohpc-ju.europa.eu/documents/EuroHPC_RIAG_Strategic_Agenda_2019.pdf

Unfortunately, due to the COVID-19 outbreak, the consortium had to cancel or postpone other important collaborative events, such as:

- A special MAX session "Computational Materials Science towards the Exascale: performance portability and use cases" in the frame of the EuroHPC Summit Week 2020 in Porto (March 24, 2020);
- Participation in the design and organization of the Psi-k-2020 conference (rescheduled to August 2021): a MAX dedicated booth, the organization/participation/chair in several thematic sessions, a specific MAX event after the conference closure.

The full list of events is available in Annex 3.

Along with the European HPC organizations, specifically the ones acting in the field of materials, MAX has also co-organized several training activities, especially in the field of its flagship codes. A full list of training events is given in D8.2. In addition:

- MAX members have participated in the European HPC Training Stakeholder Workshop organized by FocusCoE in Brussels, 8/10/2019 aimed at designing common training activities for the CoEs;
- One hackathon has been organized with PRACE, 3 workshops with Psi-K and 4 schools with CECAM, showing the collaborative network of MAX in the European ecosystem.

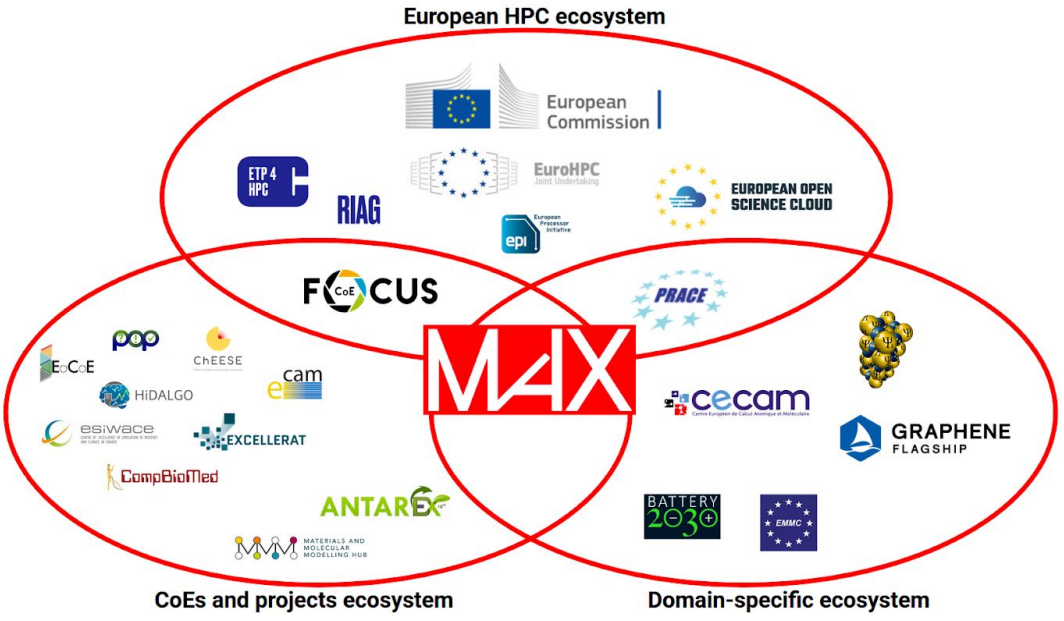


Figure 5. A representation of main MAX *synergies in the European HPC ecosystem.*

3.4.2 Industry

In this paragraph we address industrial companies organized according to different categories:

- Commercial developers of materials simulation software (also named independent software vendors)
- Industrial end users of materials modelling in small and large European companies
- Hardware manufacturers and integrators

In general, industries benefit from MaX impact on codes and platforms, for which we refer to in Sections 3.1.1 and 3.1.2. Importantly, it was often emphasized by industry that finding skilled personnel is their major bottleneck, so MaX contributions to training and education of students and young researchers is perceived as very relevant.

Independent software vendors (ISVs) interested in MAX are companies operating in the broad materials, chemistry, pharmaceutical and biotechnology domain. As MAX operates with open source software licences, they can have free, direct access to MAX codes and have especially gained from the modularization activities performed by MAX.

All the ISV companies in contact with MAX expressed interest in code integration, support and face-to-face training. MAX found an effective route of collaboration starting from its High Level Consulting Services and training, and two significant agreements were signed (see Table 2). More specifically:

- several services (D10.2 - Appendix 2): 5 code and simulations consulting meetings, 4 code development meetings, and 4 materials discovery consultations;
- two long-term signed contracts for face-to-face industrial training users (D8.2 - paragraph 3.4)

Industrial end users of computational materials modeling and design are typically manufacturing companies (large, medium and small) covering several sectors and materials categories, from consumer goods to industrial chemicals, from polymers to alloys etc. Among the MAX outcomes, they are interested in the use of flagship codes and workflows, and also in high level consulting and training. Some of the impact of MAX towards these companies is sometimes brought through the support of independent software vendors. Direct impact is witnessed by the following data:

- more than 30 industries have had a business contact with MAX partners, half of which ended in a contract. A list of commercial contracts from 2018-2020 is given in Table 2 for income of approx 240K €; several amounts have not been disclosed.
- more than 24 person-days have been delivered to industrial end users by different MAX partners, and 120 more are due (See D8.2 "First report on Training and Education"). Experience has shown that industrial users are not attracted by the school format; they prefer the "face-to-face" training that is strictly and specifically related to the needs of the customers and explicitated in the contracts.

Among the actions performed to increase MAX impact on industrial users we highlight:

- participation in conferences with industry-oriented talks and audience (about 10 from different MAX partners, complete list in Annex 4), e.g. the "EMMC Workshop on Industrial impact of materials modelling – achievements and perspectives" (8-10/07/2019, Turin: 70 experts involved or interested in the development of materials science, including end-user

and ISV representatives); Cineca & Prace workshop: HPC for Industry 4.0 (21-23/05/2019: presentation about "MaX: screening and designing materials with HPC"; 37 speakers of which 30 from industry and others form institutions and academia);

- organization of the MaX Webinar "Industry and Materials design at the eXascale: bridging the gap", 4/9/2019. The webinar was attended by 60 people from industry and academia. It is still available on the MAX website for consultation.[14]
- participation in specific working groups and activities coordinated by the FocusCoE CSA
- last but not least, a large number of direct business contacts between MaX partners and industries, which have turned out to be the most effective channel towards actual contracts of economic relevance.

Initial MaX contact / contract	Year	Type of service	Short description of the activity/service provided	Customer business area	Duration of activity/ service (months)	Revenue (K€)
BSC	2018-2019	Consulting	Consulting about atomistic simulations	Manufacturer / end user	12	120
BSC	2018-2021	Code development	Code optimization	Hardware manufacturer	36	330
CINECA	2019	Consulting	Car-Parrinello simulation setup, test and optimization of a small protein in water	Manufacturer (end user)	4	10
CINECA	2019	Consulting	Car-Parrinello simulation setup, test and optimization	Manufacturer (end user)	2	5
EPFL	2019	Materials discovery	New solid-state electrolytes	Chemical Industry	24	ND
EPFL	2019	Materials characteriz-ation	Ferroelectrics	Electronic industry	24	ND
EPFL	2020	Materials discovery	Qubits	ICT		ND
ICN2	2018-2019	Consulting	Atomic modeling of oxygen mobility in materials for oxygen sensors	Manufacturer (end user)	24	ND
ICN2	2019-2021	Consulting & training	Consulting about the use of SIESTA for the study of topological insulators	ISV		70
CNR	2019	Training + Support	Training; support concerning QE+QM/MM	Manufacturer (end user)	12	25
CNR	2019	Code development	Consulting/code development	Hardware company	18	17
SISSA	2018-2019	Code development	Software on demand	ISV	24	110

[14] http://www.max-centre.eu/webinar/industry-and-materials-design-exascale-bridging-gap

SISSA	2013-2018	Code development	Study of materials modelling	Food company	60	130

Table 2. List of commercial contracts by MaX partners in 2018-2020.

We finally discuss the category of **hardware manufacturers.** They collaborate with MAX in several co-design actions, which aim at supporting the needs and evolution of materials domain applications in synergy with the evolution of HPC architectures and software. Productive collaborations have been strengthened, as reported in the deliverable "D4.4 First report on co-design actions".

From a technical perspective, the main collaborations involve:

- NVIDIA, which officially supported the QE porting on GPUs, producing the QE v6.4, able to run on systems based on hybrid MPI + GPU acceleration on architectures based on the NVIDIA GPUs. This release can be considered an important starting point for alternative and future hybrid-architectures.
- Fujitsu, Marvell and ARM are involved in testing code refactoring on different architectures (ARM+GPU and ARM+SVE), also relevant for what concerns the EPI program.
- Intel, with one unit of personnel allocated at CINECA, has contributed to the testing and porting of some of the MaX libraries (e.g. FFTXlib) on Intel accelerated HW using the oneAPI framework.

The dissemination of MAX efforts in co-design took place mostly through:

- more than 10 events at pan-European and international level in which more than 8 MAX members participated and communicated to a medium expert- and advanced- public how to exploit HPC architectures and refactored MAX flagship codes (e.g. SC19, HiPEAC2020, PASC19, CODES@OEHI Hackathon in collaboration with EPI).
- the ARM research webinar on key ARM technologies in two episodes organized by MAX on April 16 and 18, 2019.

Collaborations with hardware companies has often brought significant support to MaX, mostly in terms of

- in-kind contribution to MaX code development, hackathons and training: a rough estimate amounts to at least 50 person days of high level experts in the first half of MaX;
- allocation of expert work co-located with the HPC Centres.

3.4.3 Research and academic institutions

The largest impact on research developed in public institutions and universities comes from the advancements produced by MaX in codes, information and data platforms, and services: for these we refer to the previous paragraphs.

Dissemination towards this sector typically occurs through publication of papers and participation in specialized conferences. The specific scientific and technical publications by MaX members are listed in Annex 2, and regularly updated on the MaX website at http://www.max-centre.eu/publications. The scientific and technical conferences where MaX members have given presentations is in Annex 4

(in addition, MaX partners gave many scientific talks showing research based on MaX codes and acknowledging MaX, not reported here).

In addition, MaX has co-organized and/or supported a number of scientific and technical workshops and events. The most relevant conference for MaX is the Psi-k-2020 conference, and referenced in the GA, which typically involves over 1000 computational scientists in the field of materials (currently rescheduled to August 2021, see https://www.psik2020.net), but three additional workshops on specialised scientific topics using frontier HPC were co-organized with Psi-k, and three more are expected in the coming year (pending Covid-19 rescheduling).

Schools and training initiatives are a key vehicle also for dissemination of the MaX outcomes towards scientists in academic institutions, besides their main impact on education. In deliverable D8.2, we thoroughly describe all the training activities done up to M18. The stakeholders represented by industrial & academic code users and developers are the main target of these. In the past months, before and despite the pandemic, MAX directly organized events that gathered more than 300 participants in the following summarized events (for more details, Table 1 and related sections in D8.2):

- 6 Schools organized for flagship code users (3 effectively took place, 3 are converted to virtual editions because of the pandemic) on the usage of pre-exascale machines, including hands-on sessions. 2 more schools have already been planned.
- 5 Hackathons and workshops on training a new generation of code developers. 2 more hackathons have already been planned.

The general feedback of the quality, training materials and organisation was on average very high and positive - 4.7/5 based on the MAX feedback form and evaluation criteria (for more details refer to D8.2).

Another important and relevant part of MAX training are the teaching modules in Universities. This action is a direct contribution to European and international Universities having in their Master and/or PhD programme courses on materials science, computational modeling and HPC. This was reflected in 4 Master programme contributions - involving a total of 57 students - with introductory courses for undergraduate students on computational materials science, hands-on sessions on usage of MAX flagship codes and best practice in their usage in HPC facilities.

Finally, master and PhD students as well as postdocs demonstrated a very high interest in one-on-one training, which MAX organizes by hosting academic and industrial researchers in CoE laboratories, for scientific projects involving the use of MAX flagship codes. In the past 18 months, more than 30 researchers were hosted at the labs with basic and specialized training on MAX codes and libraries.

3.4.4 The general public

Though MAX core activities are very specific and extremely technical, several efforts have been made to design and deploy enhanced dissemination towards society, with the purpose of introducing the general audience to materials modelling and the new exascale technology.

First of all, MAX renewed last October 2019 its website (see details in section 5.1.1), creating a page dedicated to a new and non-expert public, that is easily reachable clicking on the About link. The concepts underlying MaX are explained in a simple way not to scare the curious but unaware reader (http://www.max-centre.eu/general-public).

Furthermore, a story-telling video was recently produced to help the viewers in creating a frame for the materials discovery importance and the connection existing with supercomputer power. It shows how MAX is creating ready-to-use solutions with multiple services for their existing and prospective users from science to industry, starting from fundamental physics, model approximations and computational algorithms. The video will be referred to in the website, and will be available in the MAX youtube channel (https://www.youtube.com/watch?v=do3Q68BibY0).

Direct interactions with the general public and activities of dissemination/outreach were performed during European researchers night on September 27, 2019 by several partners: e.g. one dedicated stand in Trieste (SISSA) and one in Modena (CNR).

Finally, a dedicated session on "Supercomputing and the science & technology of the future" for the general public was co-organized by MaX in the European Open Science Forum (ESOF, https://www.esof.eu/en/), and is now being rescheduled to 2-6 September 2020 owing to the Covid-19 pandemic.

4. Impacts from Stakeholder Engagement Events

In this section we review the individual measures that allowed us to obtain the above mentioned impact.

4.1 MAX Training Events, Hackathons and Workshops

As anticipated above, and detailed in D8.2 (First Report on training and education), MAX WP8 has implemented a busy training and education programme at the pan-EUropean level, spanning from schools, to tutorials, hackathons and workshops. The level of training varies according to stakeholder, who, for the training and education program are: a new generation of code developers (goal "filling the pipeline of new generation code developers" under T8.1); academic and industry code users (advanced training); Master students; researchers receiving on-site training. MaX activities in training are often organized with other EU institutions, in a common offert to reach out to the materials modelling community.

MAX organized (with partner institutions such as CECAM, PRACE, Psi-K):

- 6 hands-on schools organized for **flagship code users** + 2 more planned
- 5 Hackathons and workshops on training a **new generation of code developers** + 2 more planned

for a total of 293 students trained in presence before the pandemic outbreak.

MAX participated in:

- 4 Master programme contributions for **undergraduate students**.

- training through research: 38 **researchers** hosted at the labs with basic and specialized training on MAX codes and libraries.
- 8 contributions to schools and training events organized by other institutions through synergies established with 314 students.

MAX online:

- 23 training events available online: tutorials and video libraries[15].

4.2 MAX Webinars

Much like the virtual training events, MAX webinars are a real asset when it comes to extending the reach across a wider pool of stakeholders, not just a necessary step in the face of COVID-19. Stepping up on the number of webinars for the period 2020-2021 has been chosen as one of the main tools to promote the thrilling results of flagship codes porting and the advancement towards pre-exascale. Webinars, which came very handy due to the period, have the beneficial factor of lowering engagement barriers with those hard-to-reach segments with little knowledge of the role of MAX in advancing materials science and HPC in general.

Uptake: **4** webinars related to flagship codes and industrial uptake broadcasted with **415** online participants (559 registered participants). 3 more in the MAX Code Webinar series are planned.

Title, Date (Q-year)	Main outcomes	Audiences Reached
ARM SVE and tools for HW-SW co-design[16] Q2-2019	Coverage of key technologies: ● Arm Scalable Vector Extension (SVE) and the open-source gem5 simulation environment. ● Arm Instruction Emulator (ArmIE) and associated methodology to evaluate the impact of SVE in the absence of SVE-enabled hardware).	Participants: 33 Computational scientists; Domain experts. Software engineers developing HPC codes
Industry and Materials Design at the eXascale: bridging the gap[17]	● 3 Use cases (QE; ICN2; CINECA) showing how industry can adopt for	Participants: 61 Industry players, including SMEs; industrial researchers

[15] http://www.max-centre.eu/training-material-related-max-flagship-codes; http://www.max-centre.eu/open-online-courses-and-videolectures; https://www.youtube.com/channel/UCcoGe0aUy4gDVRNgjQlVf3g?view_as=subscriber.
[16] http://www.max-centre.eu/webinar/arm-sve-and-tools-hw-sw-co-design.
[17] http://www.max-centre.eu/webinar/industry-and-materials-design-exascale-bridging-gap.

Q3-2019 Trust-IT with code leaders and EMMC	materials designs and development. ● EMMC insights on whitepaper outlining strategies to engage in Materials Modelling.	in materials science and modelling. Practitioners in materials science and modelling HPC and HTC Members of the scientific community.
How to use Quantum ESPRESSO on new GPU based HPC systems[18][19] Q2-2020 Trust-IT with SISSA, CINECA, CNR Nano	● Status and features of QE running on GPU based systems. ● Optimal QE usage on heterogeneous HPC systems. ● Compiling and tuning up QE for GPUs – tools and libraries needed.	Participants: 282 registrants (194 attendees) Quantum ESPRESSO users and users with allocated compute time on heterogeneous HPC systems (PRACE, ISCRA, etc...).
Managing, simplifying and disseminating High-Throughput computational materials science with AiiDA, AiiDA lab, and the Materials Cloud Archive[20] Q2-2020; Trust-IT with EPFL	● Convergence of HPC, high throughput and high-performance data analytics. ● Stand-out features and functionalities of AiiDA and the Cloud Materials Archive. ● Significant improvements and execution time for research.	Participants: 183 registrants (127 participants), 63 attendees of the QE webinar. Scientists, Researchers and students of computational scientists interested in how to automate workflows while increasing the reproducibility of their work.

Table 3. List of MAX Webinars

Main impacts:

- Continuous training: ensuring access to the webinar recordings and presentations afterwards.
- Extending outreach to existing and prospective users of MAX products and services.
- Broadcasting exascale capabilities for materials science.
- Showcasing key features and functionalities of AiiDA and the Materials Cloud, with practical information and how to get started.
- Practical guides and added value of the flagship codes.
- Using the virtual events as a launchpad for new releases, e.g. the 2nd release of the Materials Cloud Archive in May 2020.

[18] http://www.max-centre.eu/webinar/how-use-quantum-espresso-new-gpu-based-hpc-systems.
[19] http://www.max-centre.eu/events/webinar-how-use-quantum-espresso-new-gpu-based-hpc-systems.
[20] http://www.max-centre.eu/events/max-webinar-aiida.

- Gaining insights into current and potential usage of MAX products and services through online polls during the webinars (from April 2020).
- Sharing answers to participant questions through the interactive Q&A feature (from April 2020).

To offer a quantitative idea of the wide impact such outreach actions have, below we present an analysis of participants as of geographical coverage and stakeholder groups. Participants come from 44 countries: 17 EU Member States and 27 Non-EU/global. For EU27, Italy is by far the most represented country, followed by Germany, France and Spain.

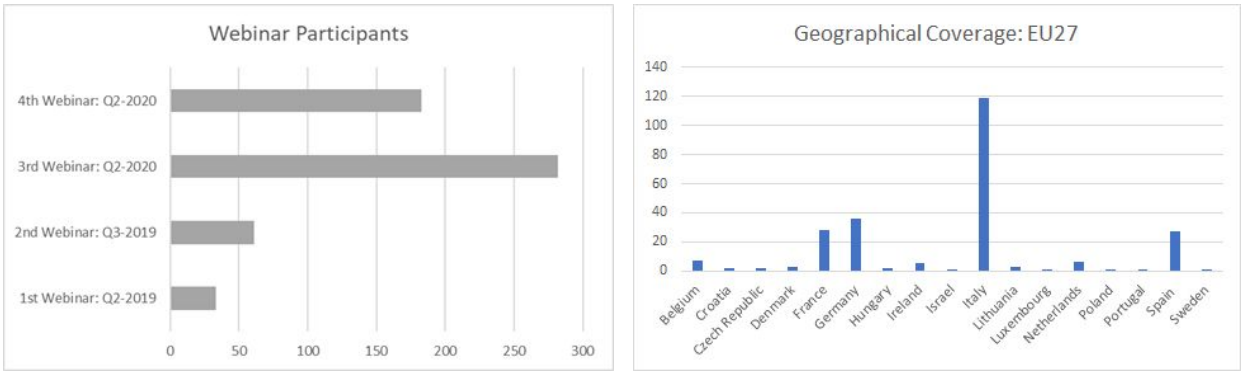


Figure 6. Total Number of Webinar Participants (left); MAX *Webinars – EU Country Coverage (right)*

Global and Non-EU 27 participation is particularly strong in Switzerland (43), UK (30), US (19) and India (15), though the overall global coverage reveals a strong potential for a European supercomputing infrastructure, code usage and development.

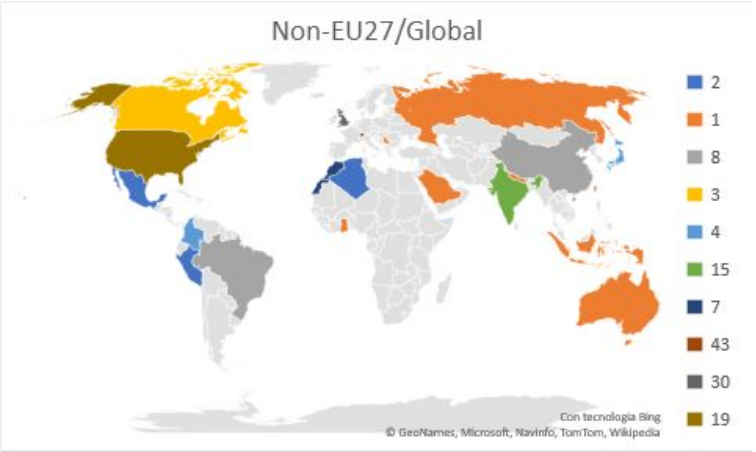


Figure 7. MAX Webinars – Global and Non-EU 27 Country Coverage

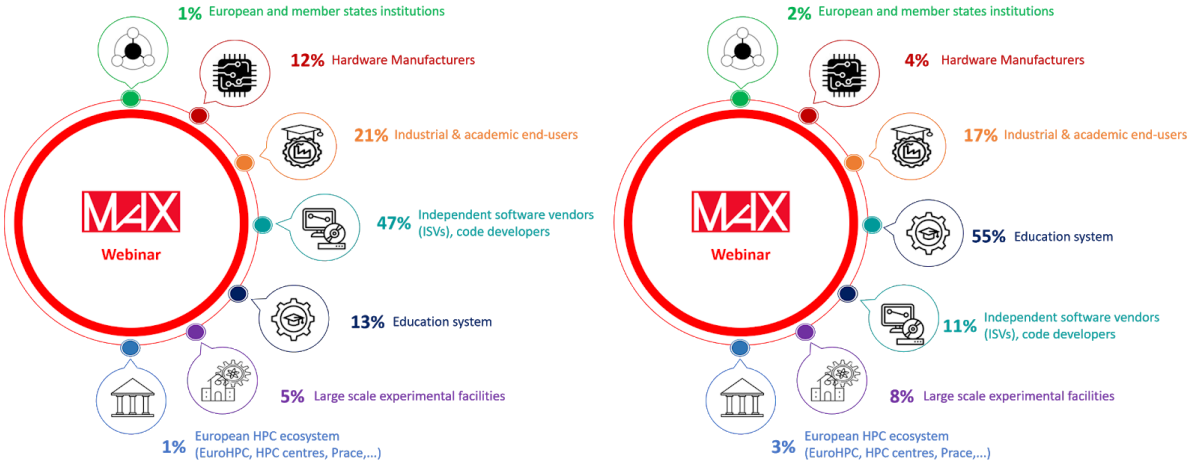


Figure 8. MAX *Webinar participants categorised per stakeholder*

The figure above shows the breakdown of participants for webinars 1 and 2 (left) and 3 and 4 (right). In Annex 5 we report the analysis of Stakeholder viewpoints, as an outcome of the 3rd Webinar, to show an insight on participants' engagement.

4.3 Third-Party Events

MAX has taken part in 35 3rd-party events since the start of the project at national, European and international level, which fall into four main categories: the HPC ecosystem, including open science and emerging technologies; materials science, including relevant HPC industrial events; women in STEM; policy and funding.

Main outcomes:

- Cluster 1: HPC ecosystem: 14 events, including major events in the field.
- Cluster 2: Materials Science: 13 events.
- Cluster 3: Women in STEM: 3 events.
- Cluster 4: Policy and funding, including collaboration with the CoEs and FocusCoE: 5 events.

All the events are listed below in Annex 3, and a list of the 32 given by MAX speakers is also given in Annex 4. Out the many events, we highlight the outcomes and impacts of selected events:

- The **PASC19 Conference 57** Platform for Advanced Scientific Community (12-14 June 2019, Zurich).

  International and interdisciplinary event under the theme of Exascale and Beyond, attracting academia, research labs and industry for an exchange on scientific computing, computational science and the use of HPC.

- ICN2: contributed to the session on "Chemistry and Materials" and gave an overarching introduction of MAX during the conference.
- CINECA: submitted the Mini-Symposium on "Exascale co-design for European Flagship Materials Science Codes".

- **Graphene Week 2019** (23 September 2019, Helsinki)

  Europe's leading conference in the field, attended by **200 experts** from **academia and industry**.

  - Elisa Molinari (Coordinator, CNR)acted as co-chair of the session entitled "**European HPC initiatives and 2D materials research: Collaborating and Funding Opportunities**" [21]. This session explored upcoming advances and potential challenges in 2D materials research enabled by HPC.
  - E. Molinari and Vladimir Falko, Director of NGI, chaired a **Graphene Flagship – MAX joint workshop** was organized on "High-performance computing for 2D materials research", with a Parallel Session and a Poster Session on 24/09/2020.

We also point out that, in Annex 3, the table A3.3 lists the events that have focused on rewarding and incentivizing women in STEM; good examples of female participation include *the Summer School on Advanced Materials and Molecular Modelling with QE* (September 2019) and the *Computational School on electronic excitations using the Yambo code* (January 2020), as first steps towards increasing the number of women trained in the field. More considerations are made in Section 2.

5. Impacts of the Communication Strategy

Leveraging, in part, on the project partner networks, MAX is using various channels and producing a set of tailored communication formats targeting different stakeholder groups. A full MAX stakeholder overview is provided in D9.1 (M6) and will be updated in D9.3 (M24).

Through the use of a storytelling technique, endorsed with documented facts, the stakeholder mapping journeys grant the reader of the deliverable the perspective of the MAX stakeholders and provide practical examples of how the latter has interacted with the communication materials produced, as well as the tools and channels used as part of the dissemination and communication strategy.

5.1 Website and Social Media

Web and Social Media presence are both central elements in the dissemination activities and engagement of MAX.

5.1.1 Website

[21] https://sc19.supercomputing.org/presentation/?id=ws_canopie110&sess=sess136.

The design of the newly launched MAX website (http://www.max-centre.eu/) website offers a user-friendly browsing experience for our stakeholder community, for all the partners involved and for anyone potentially interested in the MAX project, providing an easy way to learn about MAX assets, such as software, exascale, data and services, up-to-date information and results.

The website was launched on 21 October 2019 after a complete graphical and content renewal, and has so far has had 11.1K unique visitors and 22.1K page views. The figure below provides a snapshot of the MaX wireframe with its subsequent content sections.

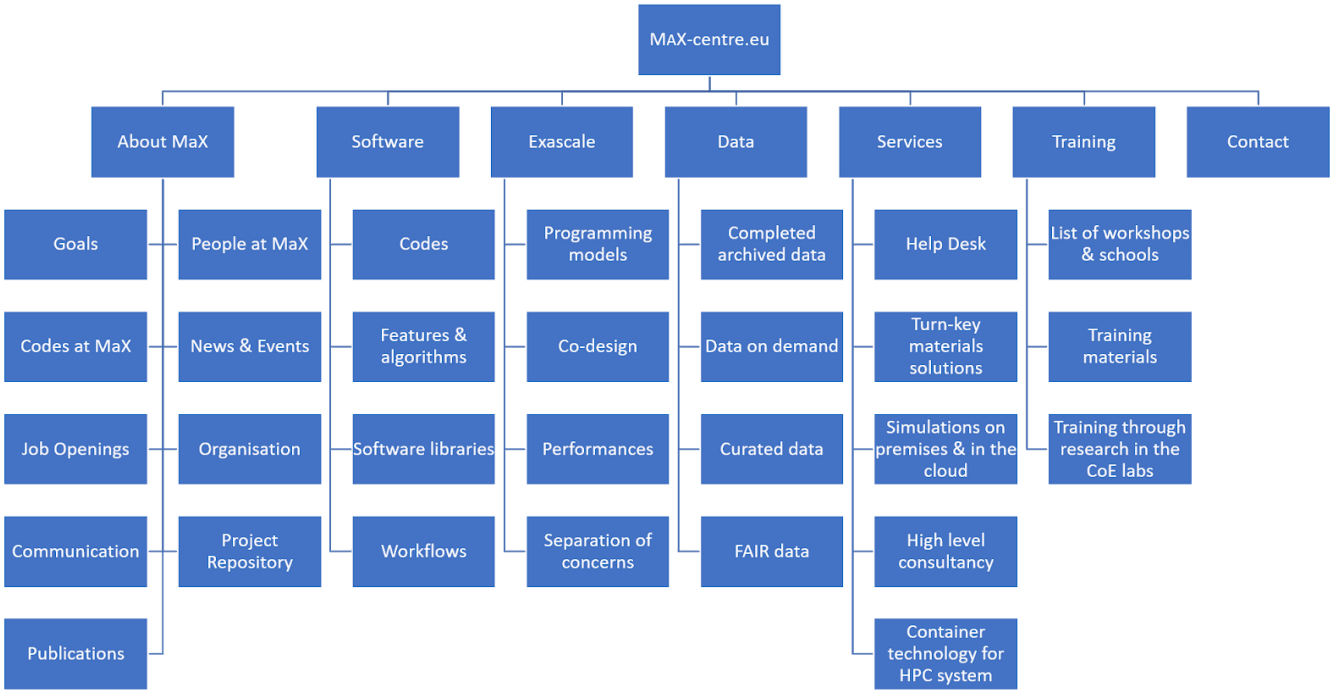


Figure 9: MAX *Website Structure – 2nd release*

5.1.2 Social Media Channels

A coordinated and regular communication through MAX social media channels (Twitter and LinkedIn) is being catered and ensured by WP9. At the moment, MAX's Twitter profile (@max-center2) counts **838 followers and 1019 tweets**, and the LinkedIn profile (in/company/max-centre) counts **239 followers and 162 posts**, showing a constant growth in numbers. The majority of the social media followers are from Research groups (35%) followed by Higher education (18.8%) and Information Technology & Services (14.5%).

	Post	Impressions	Retweet	Followers
	1019	824K	1.8K	838
	162	24.5K	89	239

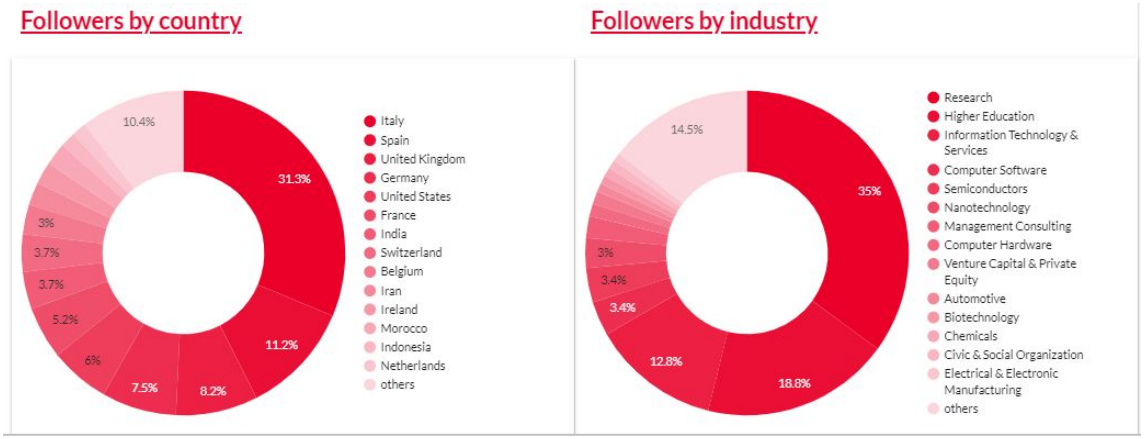


Figure 10: MAX *Social media statistics*

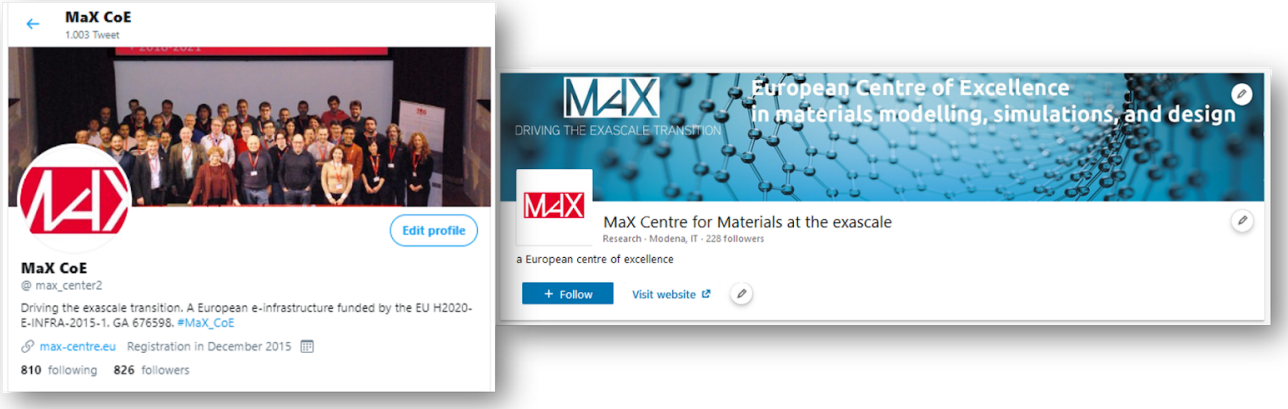


Figure 11. MAX *Twitter (left) and LinkedIn (right)*

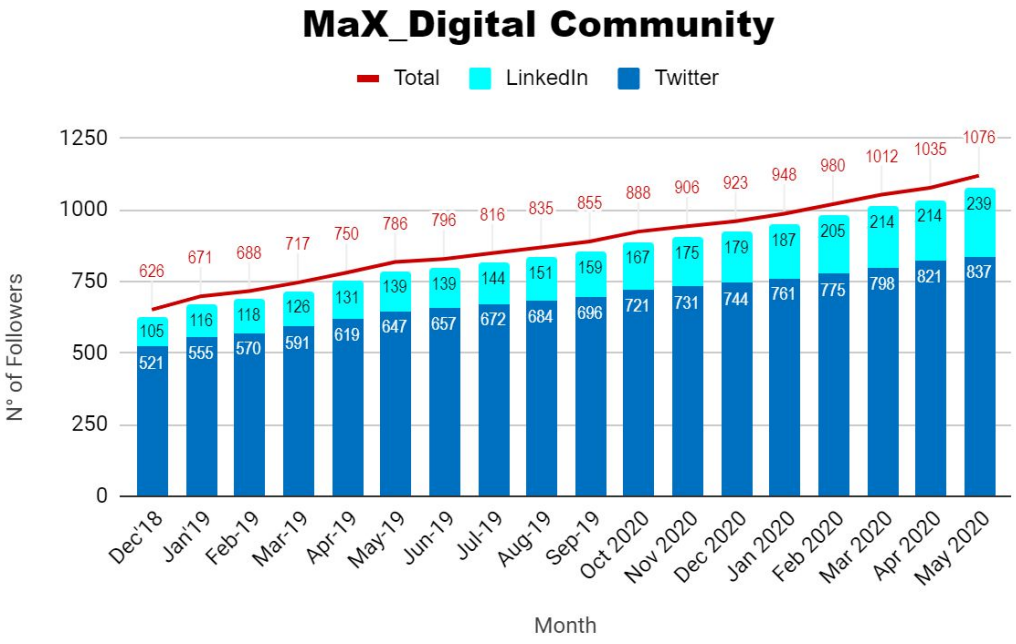


Figure 12. MAX *Twitter and LinkedIn followers – Monthly progress (M1-M18)*

5.1.3 Monitoring impact of activities

In line with the commitment to deliver a structured communication strategy, it is fundamental to monitor and measure the impact of all the communication activities carried out. As such, and for a continuous and easy monitoring of KPIs, WP9 has set up a shared dashboard (for internal usage), collecting and visually rendering relevant data from the MAX website, social media channels and online activities. Necessary adjustments will be made during the course of the project.

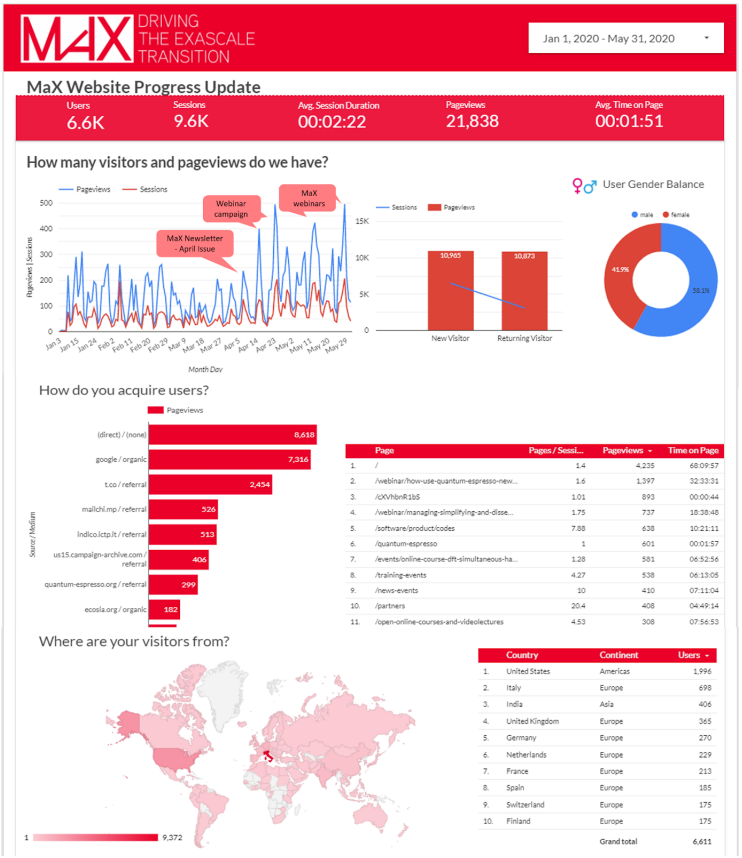


Figure 13: MAX *Dashboard examples, data covering the period from 1-30 April 2020*

The MAX dashboard was set-up by collecting data through Google Analytics and rendering it through Google Data

Studio. The dashboard is interactive and contains multiple filtering functions, so that the internal team having access to it can easily access specific and time-limited data and set up communications strategies accordingly. Data currently displayed on the dashboard includes website data as: pageviews, sessions, users, users' countries, pageviews and sessions in time, website sessions according to countries, website users' source, most visited pages and average time spent on the page; Twitter data as: followers count, tweets count, retweets, likes, specific data related to each tweet; LinkedIn data as: followers, impressions, likes, engagement and specific data related to each post.

The Dashboard is a customized analytical tool created for MAX that generates real-time information on a core set of metrics and KPIs (Key Performance Indicators). The tool tracks, analyzes and displays data about the impacts of the website and the overall performance of the project, e.g., the number of visitors, page views, new and returning visitors, gender usage, country coverage, and the most popular pages.

From the image above, it is possible to determine that the webinar pages are among the most popular pages, which is backed up by the data for the 3rd and 4th webinars, a determining factor to ensure these are continued in the coming months too. Moreover, the country visits reflect, to a good extent, the webinar country coverage, with the highest number of participants coming from Italy for EU27 and India, UK and the U.S. for non-EU27/global participation.

See below examples related to the period of MAX major activities such as newsletter issue and webinar campaign, highlighting the peak of visits, page views and geographical coverage.

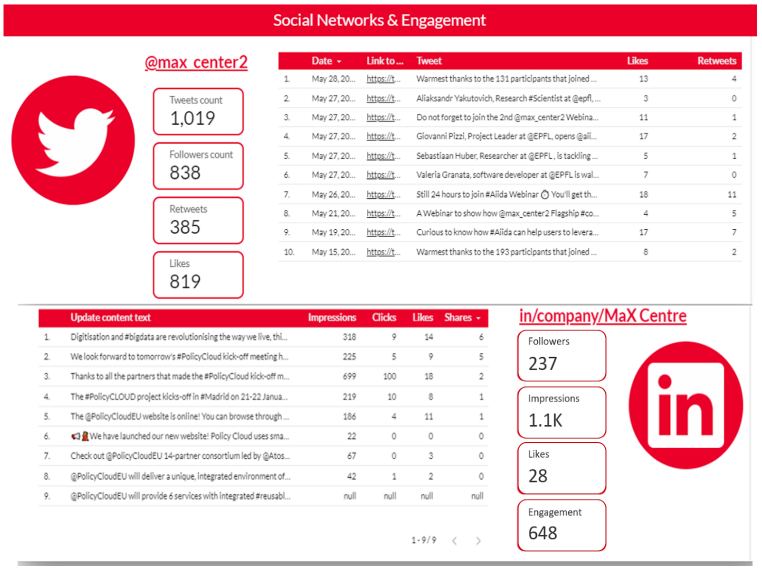


Figure 14: MAX *Social network engagement Dashboard Monitoring*

5.2 Digital Stakeholder Engagement

The MAX stakeholder engagement strategy is KPI-based with additional qualitative metrics aimed at analyzing the community in more detail, such as gender balance and examples for each stakeholder group. The table below reflects the status of the KPIs at M18 (May 2020).

From the table below, 772 are newsletter subscribers out of the 1556 total mailing list subscribers. The latest newsletter released was sent last April 2020 which gained 41% (282) open rate and a total of 153 clicks.

D9.2 Metrics	Target M12	Status		
		M6	M12	M18
Engaged stakeholders	1000	**1716**	**2137**	**3153**
• Mailing list contacts		800	1100	1556
• Twitter followers		647	732	838
• LinkedIn followers		139	175	239
• MAX Event participants		130	130	520

Table 4: KPI Status for Digital Community Interaction

5.3 MAX Digital Community and Analysis

MAX digital community recruitment campaign focuses on building the MAX engaged stakeholder contacts across the mailing list subscribers, and social media connections, followers and event participants and newsletter subscribers.

The majority of the stakeholders in the MAX community come from European countries, besides there are some HPC and scientific experts from Asia, America, Africa and Oceania, 32% of the community members are female.

Figure 15: MAX *digital stakeholder geographic distribution Mailing list contacts*

The largest participation is from Italy and Germany, respectively, followed by Switzerland, Spain and the UK. This reflects the EU-centric focus of MAX, and also countries that are particularly active in fostering the entire HPC ecosystem in Europe and internationally.

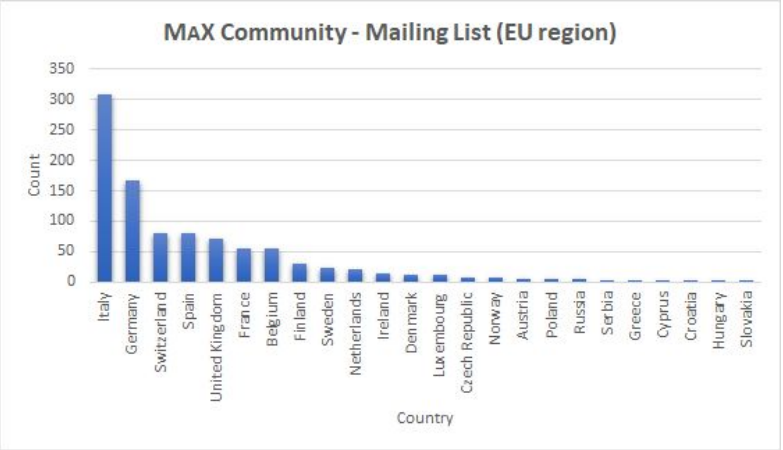


Figure 16: MAX *digital stakeholders - Mailing list contacts by country (Europe)*

The majority of the interested stakeholders are from Academia with a 42% (646/1556 mailing list subscribers) distribution count followed by Industrial and academic end-users and the EU HPC ecosystem.

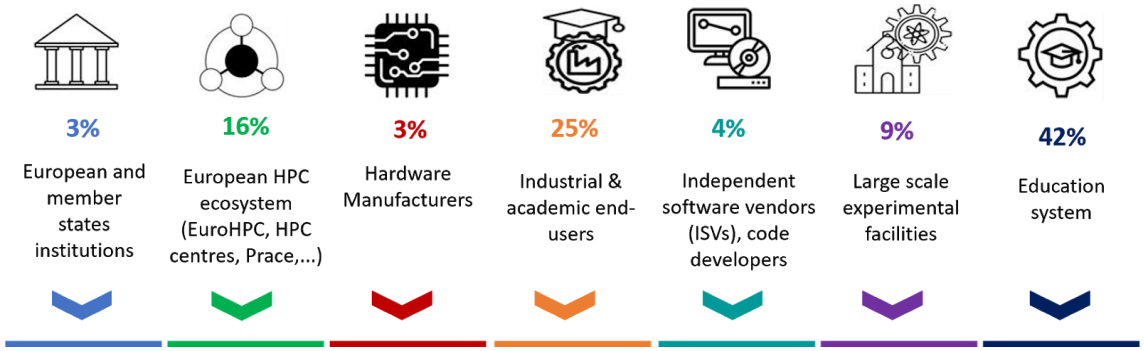


Figure 17. MAX digital stakeholder Distribution

5.4 Next Steps and Practical Plans from M19-M36

MAX is extremely active in communication and dissemination of its results, both at a consortium level and at a single-partner one. It is able to engage pragmatically, with all major stakeholders, both within the consortium and across the HPC and materials science community. At mid-term, the objective is to

consolidate further the stakeholders already engaged and focus our attention on a more general audience which is particularly challenging to achieve due to the complex subject matter. Using our communications platforms as a means to provide more testimonials from direct beneficiaries is one way to entice a more general public and obtain understanding.

Several events that were planned in training and dissemination had to be postponed due to the COVID-19 pandemic. Nevertheless, the MAX team were quick to turn the face to face events into opportunities and mitigate the situation as the whole world has had to do, to provide visibility through the flagship code webinars, as well as organising the training webinars. The consortium is encouraged that the events will be organized as a virtual format in the future or postponed to the future date. Below is a list of upcoming training events.

1st MAX video: short-term (June 2020)
The 1st MAX video has been internally designed and produced with the general public in mind, by offering a brief historical account of the importance of materials through the ages, zooming in on the upcoming revolution in materials science through exascale supercomputers and how MAX is working towards ready-to-use open-source solutions. The expected impact is to have the general aufidience able to understand the general frame of MaX assets, from materials research to the usage of cutting-edge technologies. The MaX video release will be underpinned by:

- Distributing a press release by tapping into the pool of press and media channels at our disposal.
- Carrying out LinkedIn and Twitter SMART campaigns.
- Leveraging the synergies within the HPC and materials science community to increase the number of distribution channels and boost impacts.
- Monitoring impacts in terms of visibility and coverage.

Updated communication and promotional packages: Short to mid-term (starting in June 2020)
Capture the compelling impacts of the technical developments in updated fliers and Twitter cards for circulation across the community. It is key to highlight 1) the added value of advanced computing capacities and 2) the practicalities behind the usage of MAX open-source solutions. Another vital step will be defining a full list of actions where MAX can tap into its synergies for large-scale joint dissemination.

- Updated flier on AiiDA and the Materials Cloud with practical how-to guides with 2-3 Twitter cards.
- Updated flier on Quantum ESPRESSO with a practical how-to guide with 1-2 Twitter cards.

These will be the starting point for updated promotional materials for the other codes. Main events and scientific results can have the same promotion. All kinds of stakeholders will be kept in mind when it comes to deciding campaign contents.

Large-scale Campaigns: short- to long-term
The webinars described previously were an effective example of large-scale campaigns that drew not only a varied mix of stakeholders but a relevant number of participants as well that is not to be underestimated. The consortium will draw on this and continue in the same vein for the other organised events that will be rolled-out in the coming months.

Results Brief Reports through its campaigns: mid-term

For the future content, we intend to draw on the results that provide more a "voice to the end-users" and help leave testimonials who can vouch for the results that are produced within MAX, hopefully covering all different stakeholder groups.
Press releases or newspieces will tell the reader everything they need to know with an enticing narrative covering project achievements and complex findings always keeping in mind the general purpose: to convey a message to a broader audience than the strictly technical one the project was typically referring to. The format could take on different shapes and sizes and must include items as listed below:

- Progress on the codes development
- Portability
- How MAX is approaching the exascale & through which results
- What has been the take-away for the main stakeholders?
- Providing a voice to those taking up the codes?
- How has MAX responded to some of the Sustainable Development Goals or Mission Critical items?
- Has MAX produced any policy relevant considerations?

Events Considerations

The timeline of the events below indicated have been planned with a certain rationale to help provide some results readily available for some important events taking place in September 2020. With the **ESOF2020** planned**,** the consortium sees this as an opportunity to prepare and MaX teams have planned four webinar codes in the months from May through to and July 2020, which are **Quantum Espresso, AiiDA, YAMBO and CP2K. Two** additional webinars will be carried out in September, **FLEUR and SIESTA** . This would allow for best practices and results for the webinars to be promoted directly as "demos", during the event (whether they are physical or turned into virtual ones due to force majeure). Regardless of the global pandemic, the MAX team has taken on a pragmatic approach in finding valid solutions in order to obtain the impact desired. The final webinar code on **BigDFT** is planned for October 2020.

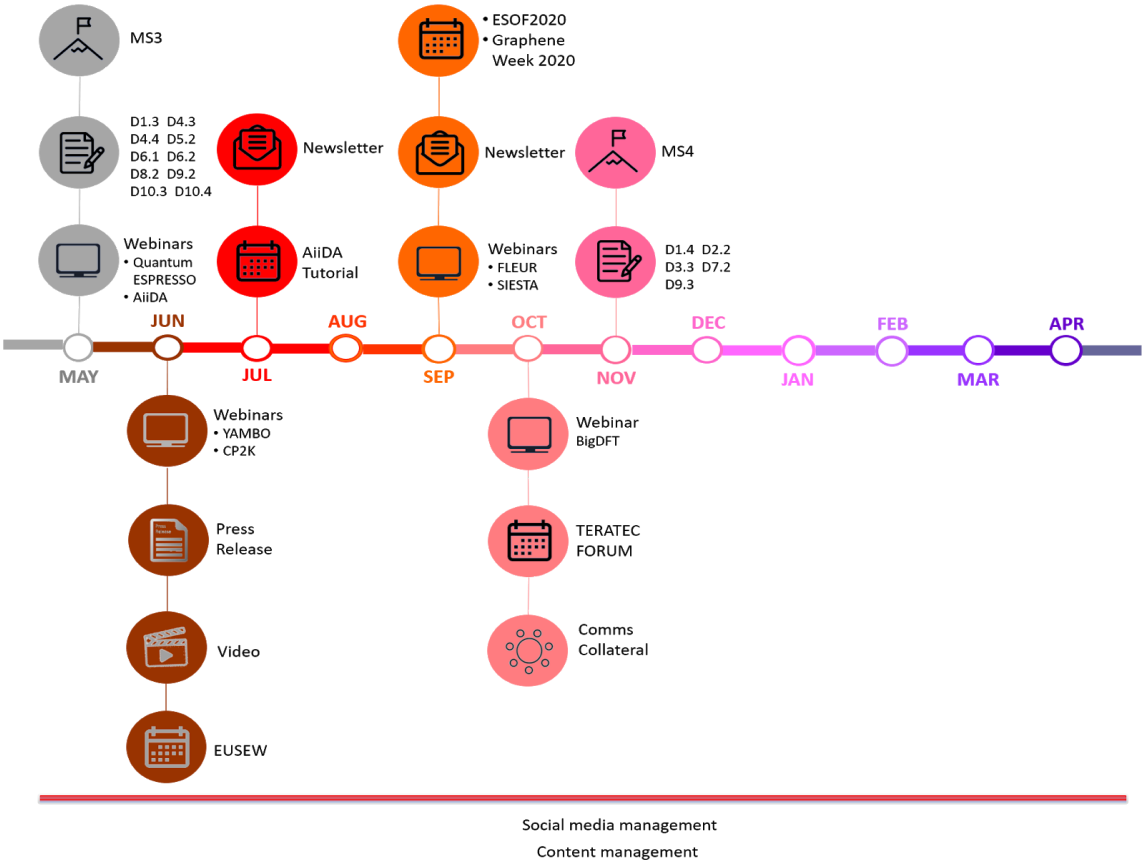


Figure 18. MAX roadmap (M18- M29)

6. Conclusions

This report illustrates the achieved impacts across the MAX targeted Stakeholders from putting into practice the Communication and Engagement plan as defined in D9.1.

The following conclusions are drawn from the experiences from M1-18:

- MAX's community is well-balanced across the range of Stakeholders.
- MAX has also established a very strong synergy with stakeholders from Academia, Research and Educational entities, which will help to increase and sustain adoption of the tools and codes moving forward.
- MAX has also managed to strengthen the relationship with a growing number of Stakeholders coming from the Industry domain, most notably from the Hardware Manufacturing and ISV field as a result of the steps taken in the first part of the project.
- Training and webinars have played a key role in building the community, giving entry to those hard-to-reach stakeholders across Europe and globally, with 44 countries reached.

This was made possible by setting up purpose-built actions and events to specifically target the needs of the abovementioned Stakeholders with a view to convey the multiple benefits of the adoption of an HPC-driven approach in the Industry scenario. MAX is now well-positioned to draw on these

experiences and lessons learnt and define a concrete set of actions defined for M19-36, including joint promotional and awareness campaigns with the established synergies. Expected outcomes will not only be the increased understanding and uptake of MAX in terms of its open-source solutions with greater emphasis on practical adoption guides but also user-centric impact reporting to policy makers and other decision makers in view of upcoming exascale computing.

Annex 1: Glossary of Acronyms

The table below lists the main acronyms used in this deliverable.

Acronym	Description
AiiDA	Automated Interactive Infrastructure and Database for computational science
CECAM	Centre Européen de Calcul Atomique et Moléculaire
CIN/CINECA	Consorzio Interuniversitario Cineca
CNR	Consiglio Nazionale delle Ricerche
CoE	Centre of Excellence
CSA	Coordination Support Action
DOI	Digital Object Identifier
EOSC	European Open Science Cloud
EPFL	Ecole Polytechnique Fédérale de Lausanne
ETHZ	Eidgenössische Technische Hochschule Zürich
EMMC	The European Materials Modelling Council
EoCoE	Energy Oriented CoE: toward exascale for energy
EPI	European Processor Initiative
ETP4HPC	European Technology Platform for HPC
EU	European Union
FAIR	Findable, accessible, interoperable, reusable
FLEUR	Full-potential Linearized augmented plane wave in EURope
GPU	Graphics Processing Unit
HPC	High Performance Computing
HPC3	HPC CoE Council (Focus CoE council)

HTC	High Throughput Computing
HPDA	High Performance Data Analysis
ICN2	Fundacio Institut Catala de Nanociencia i Nanotecnologia
ICTP	International Centre for Theoretical Physics
ISVs	Independent Software Vendors
JUELICH	Forschungszentrum Jülich GmbH
KPI	Key performance indicator
MAX-C	MAX community/EuroHPC event with MAX participation
MAX-E	MAX Event
MAX-T	MAX Training event
PoP CoE	Performance Optimization and Productivity
PRACE	Partnership for Advanced Computing in Europe
Psi-K	Ab initio (from electronic structure) calculation of complex process in materials
Quantum ESPRESSO (QE)	Quantum opEn-Source Package for Research in Electronic Structure, Simulation, and Optimisation
EuroHPC RIAG	Research and Innovation Advisory Group
SISSA	Scuola Internazionale Superiore di Studi Avanzati, Trieste
SMART	Specific, Measurable, Achievable, Realistic and Timed
SME	Small Medium Enterprise
SRA	Strategic Research Agenda

Annex 2: List of publications by MAX participants (2018- 2020)

Siesta: Recent developments and applications, A. García, N.Papior, A. Akhtar, E. Artacho, V. Blum, E. Bosoni, P. Brandimarte et al. *The Journal of Chemical Physics* 152, 20 (2020): 204108. DOI:https://doi.org/10.1063/5.0005077

Electric dipole moment as descriptor for interfacial Dzyaloshinskii-Moriya interaction H. Jia, B. Zimmermann, G. Michalicek, G. Bihlmayer, and S. Blügel, Phys. *Rev. Materials 4*, 024405 (2020) DOI:https://doi.org/10.1103/PhysRevMaterials.4.024405

Investigation of structural, electronic and magnetic properties of breathing metal-organic framework MIL-47(Mn): A first principles approach, M. Hosseini, D. E. P. Vanpoucke, P. Giannozzi, M. Berahmanf, and N. Hadipour, *RSC ADVANCES*, 10, 4786–4794 (2020) DOI:10.1039/c9ra09196c

A monolayer transition metal dichalcogenide as a topological excitonic insulator D. Varsano, M. Palummo, E. Molinari, and M. Rontani, *Nature Nanotechnology* (2020) DOI:10.1038/s41565-020-0650-4

Quantum ESPRESSO towards the exascale, P. Giannozzi, O. Baseggio, P. Bonfà, D. Brunato, R. Car, I. Carnimeo, C. Cavazzoni, S. de Gironcoli, P. Delugas, F. Ferrari Ruffino, A. Ferretti, N. Marzari, I. Timrov, A. Urru, and S. Baroni, Journal of Chemical Physics 152, 154105 (2020) DOI: 10.1063/5.0005082

Reproducibility in G0W0 calculations for solids, T. Rangel, M. Del Ben, D. Varsano, G. Antonius, F. Bruneval, F. H. da Jornada, M. J. van Setten, O. K.Orhan, D. D. O'Regan, A. Canning, A. Ferretti, A. Marini, G. M. Rignanese, J. Deslippe, S. G.Louie, and J. B.Neaton, Computer Physics Communications (2020) DOI:10.1016/j.cpc.2020.107242

Topological quantization and gauge invariance of charge transport in liquid insulators, F. Grasselli and S. Baroni, Nature Physics volume 15, pages 967–972 (2019) DOI:10.1038/s41567-019-0562-0

Theory and Numerical Simulation of Heat Transport in Multicomponent Systems, R. Bertossa, F. Grasselli, L. Ercole, and S. Baroni, Phys. Rev. Lett. 122, 255901 (2019) DOI:https://doi.org/10.1103/PhysRevLett.122.255901

Evidence for the weak coupling scenario of the Peierls transition in the blue bronze, B. Guster, M. Pruneda, P. Ordejón, E. Canadell, and J. P. Pouget, Phys. Rev. Materials 3, 5 (2019) DOI:https://doi.org/10.1103/PhysRevMaterials.3.055001

Electronic and optical properties of doped TiO2 by many-body perturbation theory, M. O. Atambo, D. Varsano, A. Ferretti, S. S. Ataei, M. J. Caldas, E. Molinari, and A. Selloni, Phys. Rev. Materials 3, 4 (2019) DOI:https://doi.org/10.1103/PhysRevMaterials.3.045401

Many-body perturbation theory calculations using the yambo code, D. Sangalli, A. Ferretti, H. Miranda, C. Attaccalite, I. Marri, E. Cannuccia, P. Melo, M. Marsili, F. Paleari, A. Marrazzo, G. Prandini, P. Bonfà, M. O. Atambo, F. Affinito, M. Palummo, A. Molina-Sánchez, C. Hogan, M. Grüning, D. Varsano and A. Marini, Journal of Physics: Condensed Matter, Volume 31, Number 32 (2019) DOI: 10.1088/1361-648X/ab15d0

Modeling heat transport in crystals and glasses from a unified lattice-dynamical approach, L. Isaeva, G. Barbalinardo, D. Donadio, and S. Baroni, Nature Communications volume 10, Article number: 3853 (2019) DOI:10.1038/s41467-019-11572-4

Prediction of Time-to-Solution in Material Science Simulations Using Deep Learning, F. Pittino, P. Bonfà, A. Bartolini, F. Affinito, L. Benini, and C. Cavazzoni, PASC19 proceedings, article n.10 (2019) DOI: 10.1145/3324989.3325720

Absolute band alignment at semiconductor-water interfaces using explicit and implicit descriptions for liquid water, N. G. Hoermann, Z. Guo, F. Ambrosio, O. Andreussi, A. Pasquarello, and N. Marzari, npj Computational Materials 5, 100 (2019) DOI:10.1038/s41524-019-0238-4

Software for quantum simulations of tomorrow, P. Giannozzi, Il Nuovo Saggiatore 35, 5-6, 34-38 (2019) NuovoSaggiatore

Fast hybrid density-functional computations using plane-wave basis sets, I. Carnimeo, S. Baroni, and P. Giannozzi, Electron. Struct. 1, 015009 (2019) DOI: 10.1088/2516-1075/aaf7d4

Coexistence of Elastic Modulations in the Charge Density Wave State of 2H-NbSe2, B. Guster, C. Rubio Verdú, R. Robles, J. Zaldívar, P. Dreher, J. M. Alonso Pruneda, J. A. Silva Guillén, C. Deung-Jang, J. I. Pascual, M. M. Ugeda, P. Ordejón, and E. Canadell, Nano Lett. 19, 5, 3027-3032 (2019) DOI:10.1021/acs.nanolett.9b00268

Guidelines for Selecting Interlayer Spacers in Synthetic 2D-Based Antiferromagnets from First-Principles Simulations, R. Cuadrado and M. Pruneda, Nanomaterials 9, 12, 1764 (2019) DOI: 10.3390/nano9121764

Precision and efficiency in solid-state pseudopotential calculations, G. Prandini, A. Marrazzo, I. E. Castelli, N. Mounet, N. Marzari, npj Computational Materials 4, 71 (2018) DOI: https://doi.org10.1038/s41524-018-0127-2

Annex 3: List of MAX organized and participated (3rd-party events)

Table A3.1

3rd-Party HPC Ecosystem Events
HPC Ecosystem Stakeholders: Supply (supercomputing centres in EU and globally, including EU CoEs; HW manufacturers; ISVs; code developers); Demand (researchers in academia and industry); policy makers (national and EU). **Total number of event participation**: 14 MAX has also contributed to several events before official project commencement with a view to securing early engagement, e.g. BDEC Conference and PRACE PCP DAVIDE OpenPower cluster: user experiences and scientific cases, both in Q4-2018.

Event	Date (Q + Year) and Location
PRACE 15th Advanced School on Parallel Computing	Q1-2019; Casalecchio di Reno (IT)
EuroHPC RIAG meeting	Q1-2019; Brussels (BE)
PRACE 15th Advanced School on Parallel Computing	Q1-2019; Casalecchio di Reno (IT)
EuroHPC RIAG meeting	Q2-2019; Brussels (BE)
EOSC-hub Week 2019	Q2-2019; Prague (CZ)
Lavoisier Discussion on Quantum Simulation	Q2-2019; Barcelona (ES)
European HPC Summit Week 2019	Q2-2019; Poznan (PL)
EuroHPC RIAG meeting and FocusCoE meeting during European HPC Summit Week 2019	Q2-2019; Poznan (PL)
The PASC19 Conference (Platform for Advanced Scientific Community; co-sponsored by ACM and CSCS)	Q2-2019; Zurich (CH)
ISC19 High Performance	Q2-2019; Frankfurt (DE)
Graphene Week 2019	Q3-2019; Helsinki (FI)
PRACE-6IP WP3 Kick-Off & HPC SIG-MarCOmms & PRACE Diversity Meeting	Q4-2019; PRACE aisbl Office, Brussels (BE)
Hands-on course "Computational Laboratory of Quantum Mechanics"	Q4-2019; Modena (IT)

Supercomputing 2019 (SC19)	Q4-2019; Denver (Colorado, US)

Table A3.2

3rd-Party Events: Material Sciences and industry Material Sciences and industry events: domain-specific and industry verticals supply and demand. Total number of event participation: 13	
Event	Date (Q + Year) and Location
Novel Materials to rethink the world @ Uniud	Q1-2019; Udine (IT)
19th International Workshop on Computational Physics and Material Science: Total Energy and Force Methods	Q1-2019; Trieste (IT)
EU project INTERSECT Kick-off meeting (Interoperable Material-to-Device Simulation Box for Disruptive Electronics): materials' modelling software and infrastructure. QE; SIESTA, AiiDA.	Q1-2019; Modena (IT)
Towards Reality in Nanoscale Materials X	Q1-2019; Levi (FI)
EMMC expert meeting on business aspects of materials modelling marketplaces	Q2-2019; Lausanne (CH)
NanoInnovation Conference and Exhibition 2019	Q2-2019; Rome (IT)
Cineca & Prace workshop: HPC for Industry 4.0	Q2-2019; Milan (IT)
EMMC-CSA Workshop on Industrial impact of materials modelling – achievements and perspectives	Q3-2019; Torino (IT)
ICIAM 2019 (9th International Congress on Industrial and Applied Mathematics)	Q3-2019; Valencia (ES)
Nanoscience and Nanotechnology	Q4-2019; Frascati (IT)
International CAE Conference 2019 (35th International Conference and Exhibition for simulation-based engineering sciences).	Q4-2019; Vicenza (IT)

Industry-research collaborations in verticals, e.g. manufacturing (e.g. Industry 4.0), automotive.	
HiPEAC 2020 (computer architecture; programming models), including industry verticals	Q1-2020; Bologna (IT)

Table A3.3

3rd-Party Events: Women in STEM

Women in STEM: events/sessions aimed at incentivising and showcasing women in research/technology.
Total number of event participation: 3

Event	Date (Q + Year) and Location
ACM Celebration of Women in Computing womENcourage 2019: Workshop on "Gendering ICT"	Q3-2019; Rome (IT)
ACM Celebration of Women in Computing womENcourage 2019: Workshop on "Data Science for Society"	Q3-2019; Rome (IT)
Materials and Scientists of the Future: The Space Girls visiting MAX CoE	Q1-2019; Modena (IT)

Table A3.4

3rd-Party Events: Policy and Funding

Policy and Funding: events on CoE collaboration, policy and funding events.
Total number of event participation: 5

Event	Date (Q + Year) and Location
FocusCoE Kick-off meeting and Workshop	Q1-2019; Frankfurt (DE)
European HPC Training Stakeholder Workshop	Q3-2019; Brussels (BE)
Digital Excellence Forum @ICT Proposers' Day	Q3-2019; Helsinki (FI)

European Research and Innovation Days	Q3-2019; Brussels (BE)
European Researchers' Night	Q3-2019; All around EU
European HPC Training Stakeholder Workshop (virtual)	Q4-2019; Brussels (BE)

Annex 4: List of talks given by MaX members

PRACE PCP DAVIDE OpenPower cluster: user experiences and scientific cases, Casalecchio di Reno (IT) @ CINECA, Italy, 10/12/2018 --- Carlo Cavazzoni, Fabio Affinito (CINECA) "The PRACE PCP in the european framework"; Fabrizio Magugliani (E4) "DAVIDE: a success story - Fabrizio Magugliani"

MolSim-2019: Understanding Molecular Simulation Amsterdam (NL) 07/01/2019 --- Daniele Ongari, Leopold Talirz, Aliaksandr Yakutovich (EPFL) "Introduction to AiiDA and Materials Cloud"

Novel Materials to rethink the world @ Uniud, Udine (IT), 08/01/2019 --- Nicola Marzari (EPFL)

19th International Workshop on Computational Physics and Material Science: Total Energy and Force Methods, Trieste (IT) @ ICTP, 09-11/01/2019 --- Nicola Marzari (EPFL) "Computational materials discovery: good data vs big data"

EMA 2020 Orlando (FL) 22-24/01/2020 --- Francisco Ramirez (EPFL) "Open Science Platform for Materials Informatics: AiiDA and Materials Cloud"

Open Science Days 2019 Berlin (DE) 02/02/2019 --- Giovanni Pizzi (EPFL) "Open Science Platform for Materials Science: AiiDA and the Materials Cloud"

Towards Reality in Nanoscale Materials X, Levi (FI) 12/02/2019 --- Zeila Zanolli (ICN2), (Invited Talk) "Spintronics at the interface"

Nano Colloquia 2019, Modena (IT) 27/03/2019 --- Andrea Ferretti (CNR Nano) "From koopmans-compliant functionals to a functional theory of the spectral density"

EOSC-hub Week 2019 Prague (CZ) 9-12/04/2019 --- Giovanni Pizzi EPFL "Pathways for EOSC-hub and MaX collaboration"

Lavoisier Discussion on Quantum Simulation, Barcelona (ES), 8-9/05/2019 --- Daniele Varsano (CNR Nano) "Exciton instabilities in monolayer T-MoS2 and bulk MoS2 under pressure"

European HPC Summit Week 2019, Poznan (PL), 15/05/2019 --- Carlo Cavazzoni (CINECA) "Grand challenge applications: technical requirements for the exascale era"; Sebastiaan Huber (EPFL) "1st European Communities Workshop on Exascale Computing Focus on High Performance Data Analytics"

HPC for Industry 4.0, Milano (IT), 21-23/05/2019 --- Elisa Molinari (CNR Nano), Fabrizio Magugliani (E4)

Nano Materials & Devices 2019 Paestum (IT) 04-08/06/2019 --- Zeila Zanolli (ICN2) “Spintronics at the interface”

PASC19, Zurich (CH) 12-14/06/2019 --- Carlo Cavazzoni (CINECA) "Prediction of Time-to-Solution in Material Science Simulations Using Deep Learning"

Optimade conference Lausanne (CH) 11/06/2019 --- Giovanni Pizzi, Leopold Talirz, Snehal Waychal, Casper W Andersen (EPFL) “Optimade implementation in AiiDA”

PASC20 Geneva (CH) 29/06 - 01/07/2019 --- Zeila Zanolli (ICN2), Carlo Cavazzoni (CINECA)

Common Format for Materials Science Data Berlin (DE) 08/07/2019 --- Giovanni Pizzi (EPFL) “Data and metadata in AiiDA and the Materials Cloud"

ICIAM 2019 Valencia (ES), 15-19/07/2019 --- Alberto Garcia (ICN2) “New features and performance”

Campus PArty Italia 3 Milano (IT) 26/07/2019 --- Carlo Cavazzoni "The energy efficiency challenge for the future of computing"

EMMC-CSA Workshop on Industrial impact of materials modelling – achievements and perspectives, Torino (IT) 08/08/2019 --- Elisa Molinari (CNR Nano) "Designing materials with HPC: the MaX European Centre"

SiSPAD - Int. conference on Simulation of semiconductor processes and devices, Udine, Italy - 3/9/2019 --- Paolo Giannozzi (IOM-CNR) “Basics of density-functional theory simulations: opportunities and limits”

MaX-Graphene Flagship joint event @ Graphene Week 2019, Helsinki (FI) 23-27/09/2019 --- Elisa Molinari “European HPC initiatives and 2D materials research: collaborating and funding opportunities”, "HPC for 2D materials research"

EPFL Open Science Day Lausanne (CH) 18/10/2019 --- Nicola Marzari (EPFL) “Project Snow White”

DACOMSIN conference Moscow (RU) 15/10/2019 --- Leopold Talirz, Aliaksandr Yakutovich (EPFL) “The AiiDA Ecosystem for Computational Materials Science”

Beilstein Open Science Symposium 2019 Rüdesheim am Rhein (DE) 15/10/2019 --- Giovanni Pizzi (EPFL) “Open Science Platform for Materials Science: AiiDA and Materials Cloud”

Grenoble-Barcelona twin conference : From quantum systems to new materials and smart electrical energy Grenoble (FR) 23-25/10/2019 --- Zeila Zanolli (ICN2) "Ab initio exciton and phonon dynamics in Transition Metal Dichalcogenides"

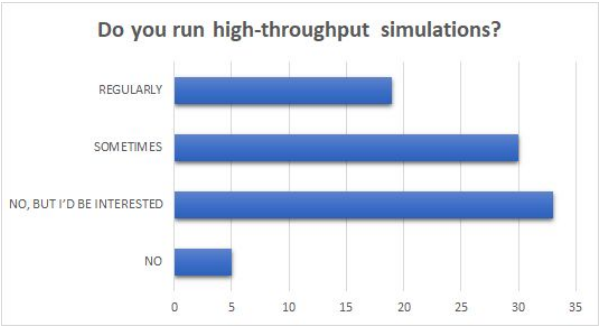
2D Materials, topological insulators and beyond Santiago de Chile (CL) 28-29/11/2019 --- Zeila Zanolli (ICN2) "Spintronics at the interface"

Symposium: Computational and Theoretical Condensed Matter Physics, Namur (BE) 17-18/12/2019 --- Zeila Zanolli (ICN2) "Spintronics at the interface"

Annex 5: Example of Analysis of Stakeholder Viewpoints

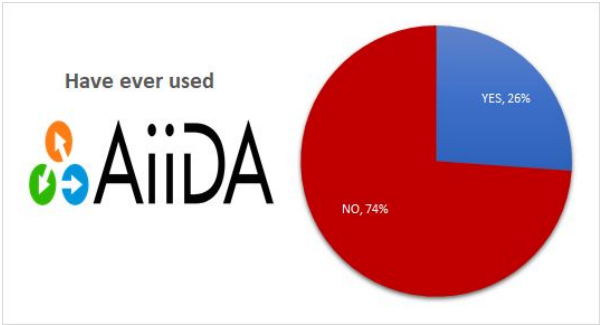
A key feature in our webinar platform is the use of **live polling** on specific questions of interest to MAX. Stakeholder engagement through webinars has therefore generated key insights on familiarity of HPC capabilities and the codes, as well as understanding trends and needs around current and potential usage. The 3rd Webinar polls (*"How to use Quantum ESPRESSO on new GPU based HPC systems*", 13/05/2020) are available online[22], while in the following we discuss results from the 4th polls to have an overview of engagement impact and show key insights in this respect from webinar 4 on AiiDA and the Materials Cloud Archive (*"Managing, simplifying and disseminating High-Throughput computational materials science with AiiDA, AiiDA lab, and the Materials Cloud Archive"*[23], 27/05/2020).

Takeaways from the 1st Poll (responses from 86/121 attendees): *There is a clear scope for increasing high-throughput simulations within the* MAX *community*. Most of the participants run high-throughput simulations, 18 regularly 30 sometimes. 33 participants would be interested in doing so.



and

Takeaways from the 2nd Poll: *There is a lot scope to increase the usage of AiiDA*. Only 26% of respondents have used AiiDA with 74% not having ever used it, showing that dedicated webinars and awareness campaigns are vital in drawing attention to stand-out features and functionalities of and other MAX products and HPC capabilities.



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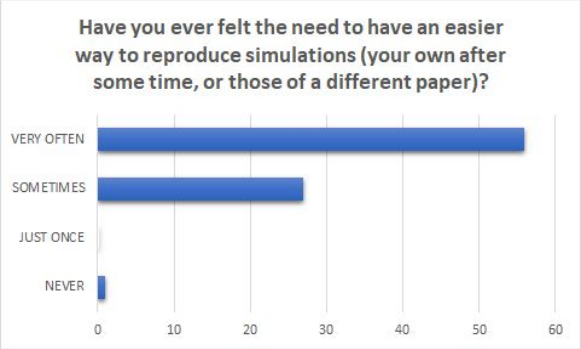
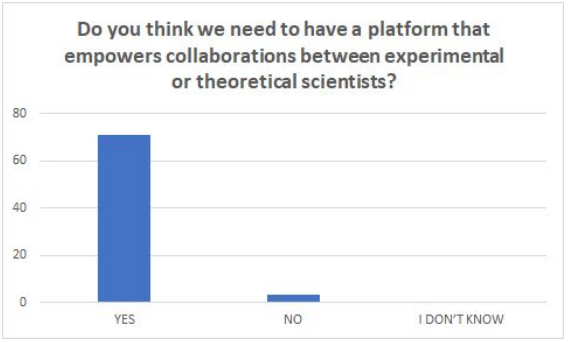
[22] http://www.max-centre.eu/news/follow-max-webinar-quantum-espresso

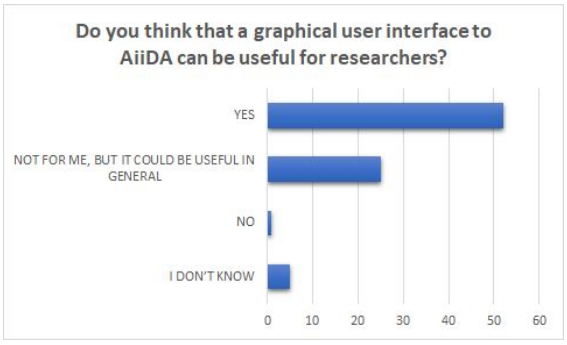
[23] http://www.max-centre.eu/webinar/managing-simplifying-and-disseminating-high-throughput-computational-materials-science-aiida



Takeaways from the 3rd Poll (responses from 84/121 attendees): *Most participants have a clear need for easier ways to reproduce simulations*, with 83 respondents stating that they regularly or sometimes have this need.

Takeaways from the 4th Poll (responses from 66/121 attendees): *There is a very clear need for a platform that empowers collaborations between experimental and theoretical scientists*. Just one respondent does not see such a need.

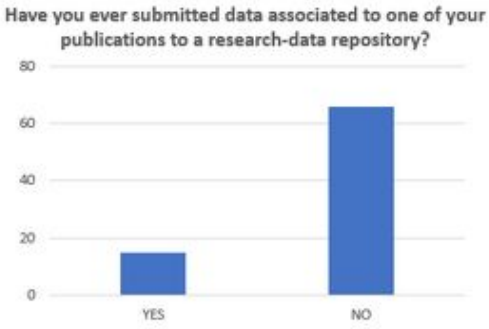


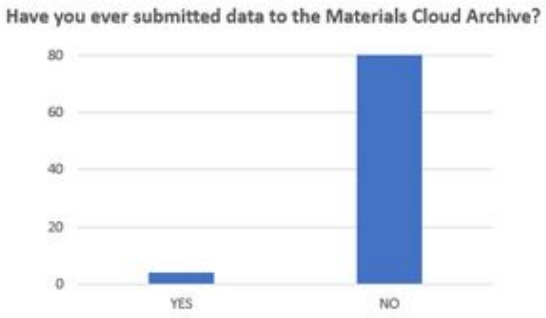


Takeaways from the 5th Poll (responses from 80/121 attendees): *Having an AiiDA interface would be useful*. 51 respondents would find it useful and 23 see it as being generally useful.

Takeaways from the 6th Poll (responses from 80/121 attendees): *Using a research data repository for publications is not a widespread practice*, at least within the sample from webinar 4, with most (62) respondents never having used one. Raising awareness of the availability of products like the Materials Cloud Archive is key to increasing usage.

Takeaways from the 7th Poll (responses from 82/121 attendees): *A very small portion of the community sampled have used the Archive*, with only 2 respondents having used it. Again, greater knowledge about it would be a key step. Actions include increasing awareness about FAIR best practices and long-term data storage possibilities as added value.





Leveraging synergies established within the HPC and EU cloud initiatives for research would be an important action to take moving forward. This could include broadcasting the "how-to video" widely across the community.

MAX has also collected feedback from end-users of its flagship codes to showcase the added value in the HPC context. The answers highlight benefits such as:

AiiDA and plug-ins: 'Screening large numbers of materials from experimental databases and running large numbers of calculations'.

AiiDA: 'The added value for industrial applications are automation, transparency and open source'. 'A powerful and flexible tool for implementing running and sharing complex workflows in industrial research'. 'Accelerating the pace of transport simulation of iron layers impurities'.

with

Example of Twitter banner for dissemination of poll results

CP2k: 'Speed and versatility for carrying out large numbers of simulations in complex systems and processes'. 'Building sophisticated chemical models; postulating and validating unique hypotheses; understanding catalysis, separations and materials'. 'Treating large atomic systems at ab-initio level for realistic models of non-volatile memory cells'.