D9.3

MAX Communication and Dissemination Strategy and Stakeholder Engagement Plan, Final version

Silvana Muscella, Julie Abergas-Arteza, Rita Giuffrida,
Francesco Osimanti, Stephanie Parker,
Maria Bartolacelli, Maria Celeste Maschio, Luisa Neri

Due date of deliverable:	30/11/2020 (**Month 24**)
Actual submission date:	30/11/2020
Final version:	30/11/2020

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.:	D9.3

Authors: S. Muscella, J. Abergas-Arteza, R. Giuffrida, F. Osimanti, S. Parker (TRUST-IT); M. Bartolacelli, M. C. Maschio, L. Neri (CNR)

To be cited as: Muscella et al., (2020): MaX Communication & Dissemination Strategy & Stakeholder Engagement Plan, Final version. Deliverable D9.3 of the H2020 project MaX (final version as of 30/11/2020). EC grant agreement no: 824143, Trust-IT, Pisa, Italy.

Content

Versioning and contribution history

Version	Date	Author	Notes
0.1	25.09.2020	Julie Abergas-Arteza (Trust-IT)	Table of Contents (ToC)
0.2	02.10.2020	Julie Abergas-Arteza (Trust-IT)	Initial Update on section 1 and 3
0.3	14.10.2020	Julie Abergas-Arteza (Trust-IT)	Initial update for engagement and stakeholder
0.4	26.10.2020	Julie Abergas-Arteza, Silvana Muscella, Francesco Osimanti (Trust-IT)	Section 1, 2, 3, 4, 5
0.5	30.10.2020	Julie Abergas-Arteza, Silvana Muscella, Francesco Osimanti (Trust-IT)	All Sections & Executive Summary
0.6	4-9.11.2020	Maria Bartolacelli, M. Celeste Maschio, Luisa Neri (Cnr)	Content proofreading and contribution to all sections
0.7	Nov. 2020	Francesco Osimanti, Stephanie Parker (Trust-IT)	Review
0.8	28.11.2020	Maria Bartolacelli, M. Celeste Maschio, Luisa Neri (Cnr)	Final review
0.9	30.11.2020	Julie Abergas-Arteza, Francesco Osimanti, Stephanie Parker (Trust-IT)	Final round of events based on final review

Executive Summary

The D9.3 "Deliverable on MaX Communication & Dissemination Strategy and Stakeholder Engagement Plan, Final version" (delivered in November 2020, M24) is the second iteration of the namesake D9.1, submitted in May 2019 M6. At the time of releasing D9.3, MAX needs to address two issues, one life-changing, the other related to boosting the content-rich approach to the plan for the period M25-36. The first aspect is connected to the COVID-19 pandemic, which is affecting everyday life, work habits and overall communication activities, obliging a fast transition towards the digital and virtual interactions. This affects the internal initiatives as well as those for stakeholder engagement and pushes us to seek for alternative means of interaction. In the second case, this updated plan explains how the communication strategy has become agile in its approach to dealing with planned activities with new formats, revised and updated plans aimed at tackling the impediments of the pandemic. Secondly, the report covers how the consortium intends to adopt impactful strategies for the remaining months of MAX with a view to ensuring maximum return of investment in terms of growing and supporting the community of users.

It is crucial that in this next phase of its communication, stakeholder engagement and dissemination strategy, we demonstrate how to make **MAX accessible to all users across Europe** with a focus on the public sector and industrial users, no matter where they are located. Under new COVID-19 restrictions, it is vital to find new forms of engagement and ways to support uptake right across the materials science the HPC and HTC, the academia and industry communities in the transition towards exascale. The updated plan therefore focuses on tangible MAX results, advances in the field, and user uptake potential through a pragmatic set of actions and clear editorial plan. In this respect, D9.3 also maps a detailed editorial plan that considers the insights indicated above in the future timeline.

To gauge progress towards the original plan in D9.1 and revisions thereof, this plan also reports a brief overview on the overall achievements to date for each activity originally defined. The plan also includes a new approach to outreach and the communications toolbox geared towards a changing landscape of uncertain evolution. Examples include a ramp-up of virtual formats, such as building on the early successes of the flagship code webinar series with a new Highlights and Insights series, a podcast series and diversified formats for MAX training.

With this, MAX assets and stakeholder benefits are foremost in mind as is the calling for an assessment of impacts for High Performance Computing (HPC), High Performance Data Analysis (HPDA) and High Throughput Computing (HTC) in the context of the MAX Centre of Excellence, its synergies and stakeholders. This more so, as new investments by the European Commission for supercomputers[1] and the transition to Horizon Europe (2021-2027) with a new framework of research fundings are upcoming. Demonstrating impacts in terms of advances and uptake will be key. In this respect, the plan is intended to pave the way for D9.4 ("Impact Assessment Report, Final Version", due in November 2021, M36).

[1] https://ec.europa.eu/digital-single-market/en/news/eu-steps-investment-world-class-supercomputers-researchers-and-businesses

1. Introduction

1.1 Purpose and Scope

This document is an update to *D9.1 MAX Communication & Dissemination Strategy & Stakeholder Engagement plan* which was submitted in May 2019 (M6). This final version (November 2020) reports on progress so far, revising original plans where necessary and defining activities for the period M25-36 (December 2020-November 2021) with a twofold objective:

1. Ensure maximum return on investment around the advances and results of MAX and the transition to exascale through a pragmatic content and community-centric approach;
2. Adapt to the restrictions around the COVID-19 pandemic in terms of stakeholder engagement by focusing on alternative but equally effective forms of interaction and reporting on results achieved.

Besides updating D9.1, this deliverable also makes reference to *D9.2 Impact Assessment Report, mid-term version* (submitted in May 2020, M18) and *D10.3 First report on MAX in the European, national, international HPC ecosystems* (submitted in May 2020, M18).

The outcomes of the plan defined in D9.3 will feed into *D9.4 Impact Assessment Report*, *final version*, which is due in M36, as a high-level overview of all the major achievements for MAX.

1.2 Adapting to COVID-19

As lockdowns have been imposed across the globe in response to the COVID-19 pandemic and activities have mainly gone digital, changing our way of working and interacting, it is nonetheless necessary to continuously monitor impacts for MAX stakeholder engagement and dissemination of results. On the one hand, MAX needs to shift its focus to its own digital formats to keep its communication and dissemination mission, such as building on the highly successful flagship code webinar series and expanded global community. On the other hand, it is important to track 3rd-party events taking place virtually in which MAX can make active contributions. Such an approach can offer a window of opportunity for effective interactions, both in terms of ensuring continued dialogue and of cost-effective, sustainable formats.

While webinars were part of the original plan, they have become a central part of MAX stakeholder engagement, enabling a really smooth transition from physical events that have been cancelled or postponed due to COVID-19 restrictions to digital ones and offering the chance of presenting cutting-edge and crucial results of MAX effort.

Best practices and lessons learnt from this experience are now feeding into the updated plan for M25-36 with the addition of podcasts, as detailed in subsequent sections.

Though taking into consideration limitations due to the current global situation, this updated plan is intended as an all-partner commitment to supporting the results and advancement of MAX according to the effort allocated. The purpose of the editorial plan is to start plotting opportunities for communicating, disseminating and engaging with stakeholders. This plan is therefore considered as a living document that allows for flexibility in the next months also following the evolution of the pandemic.

1.3 Structure of the document

The rest of this document is structured as follows:

- **Section 2:** Defines the strategy for the overall plan on MAX communications, stakeholder engagement and dissemination.
- **Section 3**: Covers MAX results and assets for dissemination and communication, spanning the flagship codes, products, services, materials cloud platform, exascale, training and training resources.
- **Section 4**: Presents the communications and dissemination plan, covering the content- and community-centric approach, visual identity and branding, liaison with training, the stepwise approach to event organisation and promotion, value proposition and messaging, visibility across the global HPC and materials science community.
- **Section 5**: Focuses on monitoring Impacts, including progress towards KPIs and targets for new measures with examples of achievements at M24.
- **Section 6**: Draws the main conclusions.

Three annexes are included:

- **Annex 1**: List of abbreviations.
- **Annex 2**: List of scientific publications.
- **Annex 3**: List of events.

2. Strategy

2.1 Objectives

MAX enables materials modelling, simulations, discovery and design at the frontiers of current and future HPC, HTC, and data analytics. Its activity focuses on six open source codes for electronic structure and quantum simulations of materials and an open-science platform for computational materials science and on their porting towards the exascale architecture. The MAX strategy for communication, dissemination and stakeholder engagement reflects the project's cornerstones in terms of the transition to exascale, flagship code advances, training and support with a focus on the user community, user benefits and service delivery.

The key purpose of the MAX's Work Package 9 (WP9) "Engagement, Communication, Dissemination & Uptake" is to support the overall project objectives in the context of best communications. WP9 is thus especially focused on ensuring that the work done within this project is brought to the attention of as many relevant partners and stakeholders as possible, actively involving them whenever possible.

The MAX communication strategy is a SMART (specific, measurable, actionable, relevant, and time-bound) and KPI-driven approach aimed at achieving a successful community building and stakeholder engagement.

The Plan is therefore aimed at establishing a mechanism which enables materials modelling, simulations, discovery and design at the frontiers of the current and future High-Performance Computing (HPC), High Throughput Computing (HTC), and data analytics technologies (HPDA) making them accessible to a large and growing pool of researchers in the materials domain.

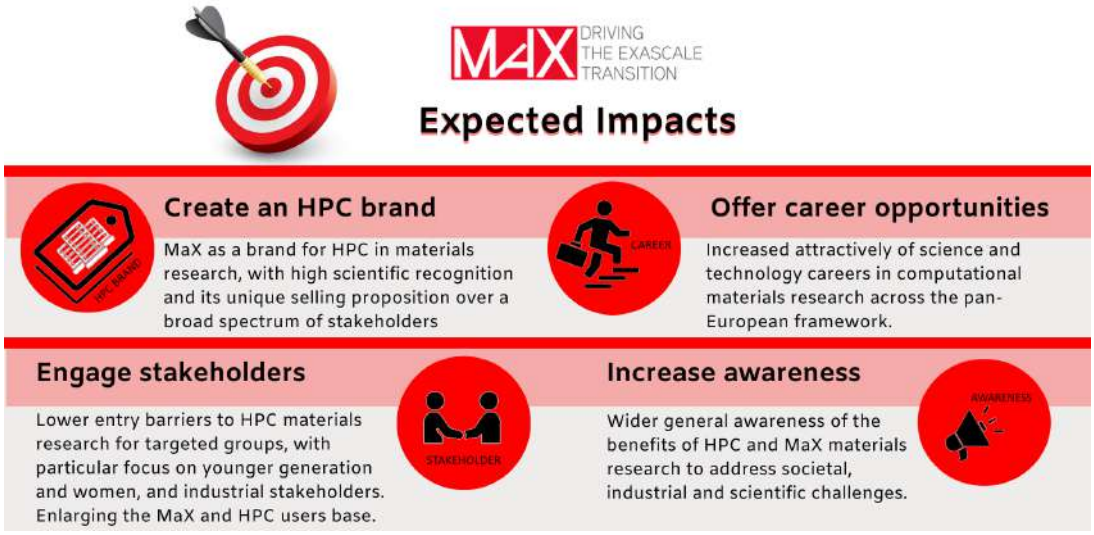


Figure 1: Main expected impacts from the strategy implementation.

These impacts are achieved through a variety of communications and dissemination activities, spanning:

- **Building an international, consolidated community** covering the stakeholders playing a role within the MAX - HPC ecosystem.
- **Implementing a multi-stakeholder engagement plan**, targeting primary stakeholders through social media channels, at MAX and external events, as well as targeting secondary stakeholders through ICT and business channels; building on existing collective networks with close interaction with the HPC centres of excellence and relevant initiatives.
- **Designing, populating and maintaining a web platform** as a highly dynamic, responsive and interactive website, and producing a variety of **branded communication material**, including, but not limited to:
    - Brochures, fliers and other collateral materials.
    - Banners for SMART promotional and recruitment campaigns.
    - Videos, including webinar video recordings.
    - Posters, both technical and non.
    - Press releases.
    - In-house newsletters.
    - Promotional articles, e.g. webinar campaigns.
- **Delivering a communication strategy**, with measurable targets, to motivate continuous activities and measure impact, including, but not limited to:
    - Community development.
    - Web analytics.
    - Social media analytics.
    - Community database profiling.
- **Producing high-quality and highly relevant content** for the MAX web platform, LinkedIn, Twitter, and YouTube channels. Creating media content on major achievements and insights on developments.
    - Editorial plans for content production.

This D9.3 brings to the plan additional formats, e.g.

- Policy Briefs designed to convey high-level impacts to policy and other decision makers in the HPC ecosystem.
- Podcasts aimed at offering insights into MAX in a relaxed and easily digestible format.

The plan is coordinated through WP9 in synergy with the consortium partners and working closely with WP8 (Training and Uptake) and WP10 (Management; especially the tasks on “coordinating with pan-European and national HPC ecosystems” and “interfacing with international HPC materials research ecosystem”) with a view to ensuring activities are highly complementary.

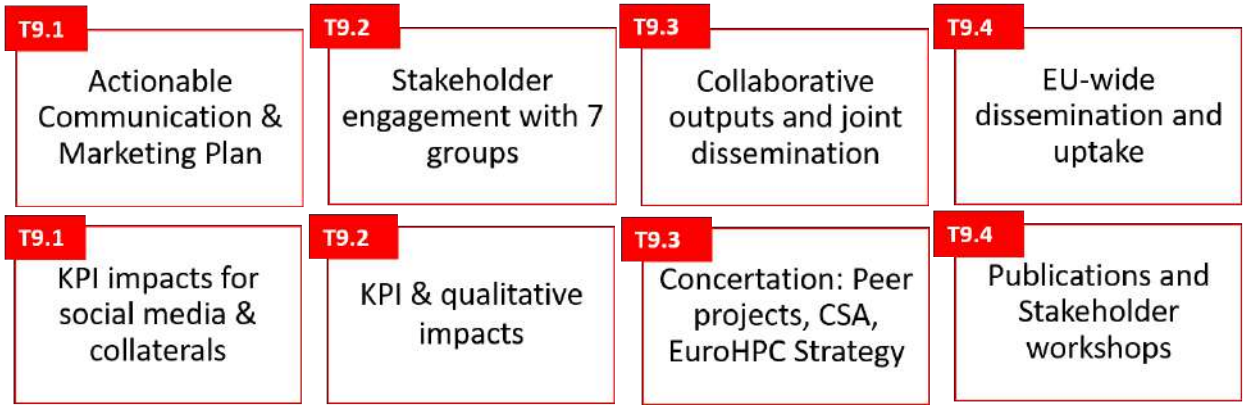


Figure 2: Activities articulated as tasks in WP9 as the building blocks to achieving uptake and impacts.

The updated plan defines the strategy for strengthened partner coordination. This entails coordinated communications and results-sharing across WPs 1-7 and continued close liaison between WPs 8-9-10 to define priorities and impact of results right across the MAX consortium.

- Intertwining the communication and dissemination activities with the results achieved across the diverse work packages with a view to telling a story on how they are linked together, which stakeholders they target and how they fit into the bigger picture.
- Liaising with WP6 on the demonstrators and in close collaboration with WP 1-5 on feedback to jointly define the overall goals and outreach plan.
- Covering key aspects of performance gains, such as energy efficiency, performance portability, to ensure greater visibility to results through interactions with relevant WPs and mapping the stakeholders targeted.
- Monitoring new scientific publications and increasing visibility around media channels through dedicated campaigns.

2.2 Stakeholders

MAX targets a variety of stakeholders in the HPC and materials science ecosystem: (1) European and member states institutions; (2) European HPC ecosystem (e.g. EuroHPC, HPC centres, PRACE); (3) hardware manufacturers; (4) industrial & academic end-users; (5) independent software vendors (ISVs), code developers; (6) large scale experimental facilities; (7) education system.
These categories have been prioritized into four main groups as per D9.2: European institutions and ecosystems; industry; research and academia institutions and the general public are the stakeholders that have the most to gain from MAX while close links to the HPC ecosystem are key for boosting impacts through synergies and joint activities, pushing the envelope for HPC and materials science. The strategy continues to tailor content and formats around the diversity of interest, ensuring that outreach and synergies are highly effective.

- **European institutions and ecosystems**: Having a major stake in advanced computing capabilities and joint contributions to the HPC strategy.
- **Industry**: Focused on creating and sharing co-design cycles for the development of new products.
- **Research and academia institutions**: Interested in accessing ready-to-use codes and using them in turn-key solutions, as well as benefiting from support.
- **General public**: Keen to learn about scientific and technological advances shaping tomorrow's society and economy from exascale to the development of innovative materials.

In M1-24, MAX has taken part in 115 events (both self organized, jointly organized with other institutions or CoEs, and third-party events). These events are grouped into four main categories: Scientific conferences and workshops on HPC, targeting mostly the HPC community and HW stakeholders (e.g. HPC centres, technology partners); Scientific conferences and workshops in materials science and engineering, physics and chemistry, targeting mostly end-users of materials simulations in industry and academia (e.g. codes & ecosystem developers); STEM and Outreach; Policy and funding, alongside training events.

The complete list of the events M1-M24 is available in Annex 3 at the end of the deliverable. Below, a summary of the events by type:

- HPC ecosystem, including open science and emerging technologies: 14
- Materials science, including relevant HPC industrial events: 48
- Policy and funding: 14
- Training: 27
- STEM and Outreach: 12

2.2.1 European institutions and ecosystems: Progress Towards Plan

The strategy for stakeholder engagement towards European institutions builds on long-term, on-going synergies with all the key players of the European HPC ecosystem:

- EuroHPC Joint Undertaking[2]
- PRACE[3]
- EPI[4]
- ETP4HPC[5]
- EOSC[6]
- CoEs and FocusCoE[7].

It is also underpinned by synergies with major players of the materials research ecosystem, such as:

[2] https://eurohpc-ju.europa.eu/ .
[3] https://prace-ri.eu/ .
[4] https://www.european-processor-initiative.eu/.
[5] https://www.etp4hpc.eu/.
[6] https://www.eoscsecretariat.eu/node.
[7] https://www.hpccoe.eu/index.php/about/

- Psi-k[8]
- CECAM[9]
- Graphene Flagship[10]

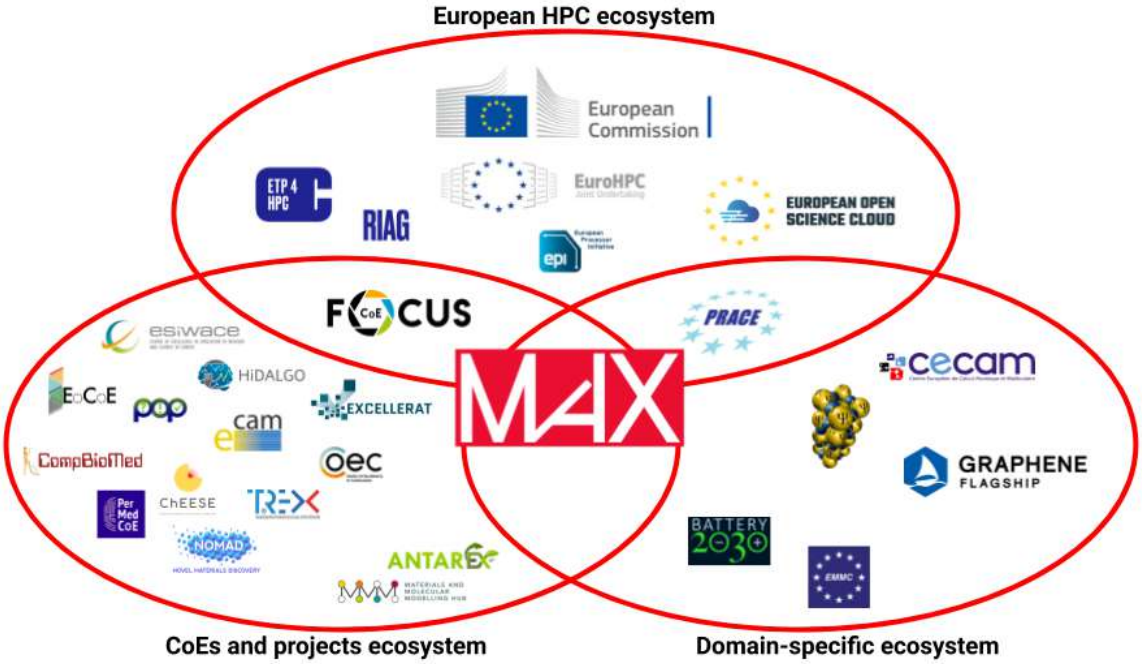


Figure 4: Pool of MAX Synergies for Stakeholder Engagement. The figure visualizes the breadth of the synergies that MAX continues to pursue as part of its stakeholder engagement.

[8] https://psi-k.net/.
[9] https://www.cecam.org/.
[10] http://graphene-flagship.eu/.

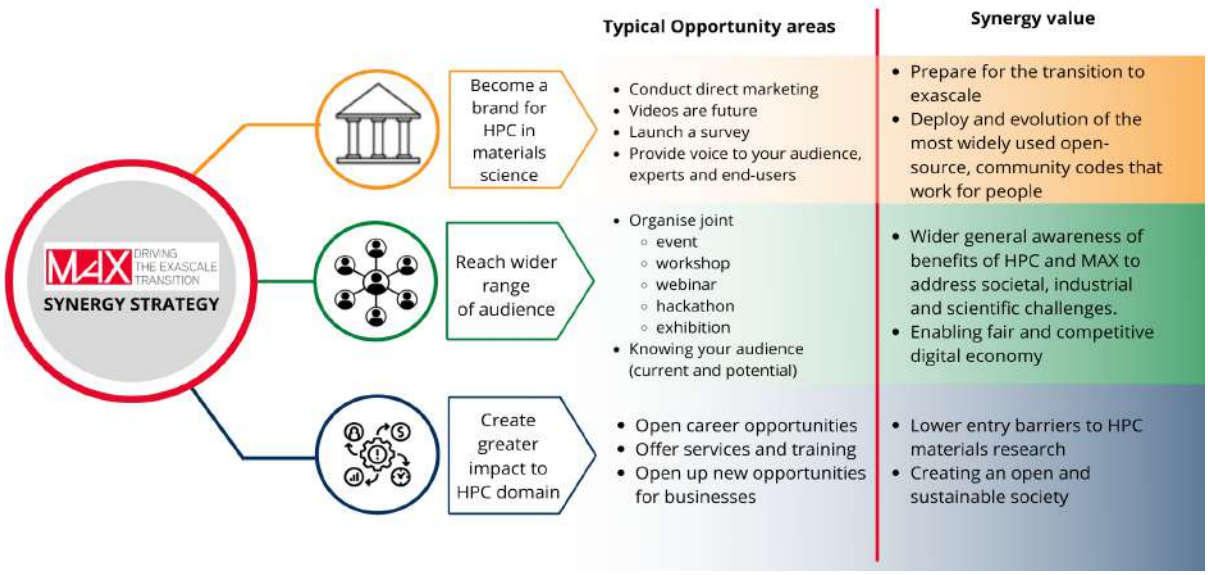


Figure 5: MAX Synergy approach for implementing above mentioned strategies.

2.2.2 Industry: Progress Towards Plan

Stakeholder engagement with industry focuses on:

- Commercial developers of materials simulation software (aka Independent Software Vendors, ISVs). ISVs interested in MAX are companies operating across the broad materials, chemistry and biotechnology domains. Thanks to the MAX open source software licences, these companies have direct access to MAX codes and can benefit from engagement and support tailored to code integration and collaboration through the MAX the High Level Consulting Services and training. Examples have been given primarily in D7.1 and D7.2, then also in other deliverables like D10.2, Appendix 2 and D8.2 - paragraph 3.4.
- Industrial end-users of materials modelling in European small- and medium-sized enterprises (SMEs and LEs). Industrial end-users of computational materials and design come from small. medium and large manufacturing companies with a focus on consumer goods, industrial chemicals (e.g., polymers and alloys), and more. Their main interest in MAX outcomes lies in using the flagship codes and workflows, high level consulting and training consolidated through business contracts with partners and through training with a preference for “face-to-face” tailored to their specific needs for the exploitation of materials modelling computing.
- Hardware manufacturers and integrators. Collaboration with MAX revolves around co-design activities aimed at supporting the needs and evolution of materials domain applications aligned with the evolution of HPC architectures and software.

Detailed impacts are reported in D9.2 (Section 3.4.2) and D4.4 *First report on co-design actions*.

2.2.3 Academia and Research: Progress Towards Plan

Public institutions and universities are a major stakeholder in terms of the uptake and exploitation of MAX, especially advancements in the flagship codes, information and data platforms, services.
As many of the partners come from this sector, on the one side this is the most natural setting for their dissemination activities. On the other hand, engagement takes place through the publication of papers and participation in specialized conferences as reported in D9.2 (Annex 2 and Annex 4), as well as through scientific talks given by MAX partners, scientific and technical workshops co-organized and/or supported by MAX.
The flagship code webinar series has also become a very important engagement mechanism for this stakeholder group in addition to schools and training activities, some of which have been impacted by COVID-19 restrictions during 2020.
The deliverable D8.2 (*First report on Training and Education*) gives a detailed description of all the training activities carried out up to M18 (May 2020), spanning academic and industrial code users and developers as the main stakeholder targets. Key achievements included physical and virtual training schools for flagship code users on the usage of pre-exascale machines with hands-on sessions and hackathons/workshops on training a new generation of code developers. Feedback forms and evaluation criteria are used to measure the effectiveness of the training materials and overall organization as a key qualitative metric.
Teaching modules in universities, by making a direct contribution to EU and international Masters and PhD programmes on materials science, computational modelling and HPC, is another element of the MAX training programme.

2.2.4 General Public: Progress Towards Plan

It is of primary importance to plan activities that involve the general public in order to raise awareness of how public money is spent, to show the success of European collaboration, and, as many members of it may be interested in scientific research, to give them the chance to understand correct even though a plain language what we do. As their main interests are often on advances, rather than technical details, MAX has focused on easily digestible messages that focus on introducing general audiences to materials modelling and the new exascale technology.

Key steps taken towards tailored engagement with this stakeholder group include:

- Creating a dedicated page on the MAX website for newcomers and non-expert members of the public, easily accessible by clicking the "About MAX" button[11]. The underlying concepts of MAX are given a straightforward explanation for anyone interested in HPC for materials science.
- Design and production of a story-telling video aimed at helping viewers grasp the key advances and concepts behind materials discovery and supercomputing capabilities. The video

[11] http://www.max-centre.eu/general-public.

shows how MAX is creating ready-to-use solutions for existing and prospective users from science and industry. The video is available on the MAX YouTube channel and has so far received 380+ views[12].

- Participating in general public events such as European Researchers' Night (2019 and 2020).

Similar and new activities will be undertaken in order to accomplish this important task.

2.2.5 Stakeholder Engagement Plan M25-36

Our plan for stakeholder engagement in M25-36 has at its core the organization or participation in different kinds of events, organized or attended bearing in mind the need to adapt to the evolution of the COVID-19 pandemic for both virtual and, when again possible, physical events. The collection of details on these events is done through a *shared event tracker* collecting all MAX- planned and participated events, by way of confirmed participation and/or (co-)organization, roles and related activities, including any papers submitted. Beyond COVID-19 restrictions, the overarching objective is to capitalize on existing networks and tailor engagement towards expanding on the MAX community in terms of outreach to the four priority groups. In order to boost the event participation results, MAX wants to implement a community and human-centric approach to showcase its value proposition through different and complementary activities and tools, e.g. designing Testimonial Cards for the social media public, increasing the number of webinars by building on the major flagship codes' success stories, and producing new engagement formats like podcasts.

Finally, it is important to consider that many of the events target diverse audiences, and MAX has the opportunity to engage with multiple stakeholders. It is important to pay attention to all of them, in order to capitalize on all the results of the Consortium: from exploitation towards policy makers to dissemination for peers, to industrial uptake. An overview of actions towards different stakeholders is given below.

- **European institutions and ecosystems**:

Objective: Carry out joint dissemination towards European institutions and ecosystems, networking all actors and acting as policymakers and huo for HPC and related projects and initiatives.
The strategy for continued engagement has a twofold objective:

- **Technical**: Interaction with a wide array of European HPC initiatives, e.g. PRACE, EPI, ETP4HPC, EOSC, Focus CoE and CoEs, new consortia for development of European supercomputers. Key activities include cooperation with these actors to share knowledge, affect and help the development of related policies.
- **Policy plans**: Sharing MAX results with board members and external stakeholders, like EuroHPC, ETP4HPC, and EOSC.

[12] https://www.youtube.com/watch?v=do3Q68BibY0&t=76s.

Premier events are a key opportunity for MAX to share expertise and acquired knowledge, also throw its own results and impact of its codes, as well as to contribute to the coordination of policy priorities. Examples include:

- **Participation in several committees of pan-European and national HPC ecosystems** to elaborate joint strategies and strengthen a synergic and collaborative network and ecosystem. E.g. role in HPC Council, EuroHPC initiatives, dissemination activities.
- **EuroHPC Summit Week** 2021 (EHPCSW; March 2021), gathers the main European HPC stakeholders, policy makers, pan-European networks and agencies, HPC infrastructures together with technology suppliers and scientific and industrial HPC users in Europe. The event is an opportunity to take forward the synergies established with the ecosystem, e.g. PRACE, ETP4HPC, EuroHPC. In the cancelled 2020 edition a MAX seminar session was planned, which will hopefully be done in 2021.
- **HiPEAC Conference**[13]: Virtual event, 18-20/01/2021. The High Performance Embedded Architecture and Compilation is a hub for European researchers and industry gathering over 2000 specialists.
- **8th PRACE Scientific and Industrial Conference (PRACEdays21; March 2021)**[14] within EHPCSW 2021, with industry presence on HPC-supported science and engineering.

In order to strengthen MAX's presence on the policy side, the aim is to continue the cooperation with external stakeholders in the HPC system. Moreover, a policy brief document is going to be elaborated and proposed to the European Commission to serve as a reference report for the HPC Consortium.

- **Industry**:

The engagement plan for M25-36 focuses on targeting industrial players with a high interest in open source codes and ad-hoc training on how to use the codes. Core engagement activities include:

- **Acquisition of know-how**: Training on open source codes aimed at increasing knowledge of HPC architecture and software.
- **Partner support**: Code development and consulting activities together with the main industrial actors.
- **Exploitation**: Help to tackle a research problem and respond to an existing demand.
- **Co-design**: Strengthening productive collaborations on co-design.

With a view to capitalize on increasing interest of the industrial sector, MAX will take part in relevant events and sessions specifically targeting this stakeholder group. The plan therefore prioritizes increased presence at industry events across Europe, whether virtually or physically throughout 2021, and including vFairs. The plan also features the MAX's showcases specifically geared towards industry, highlighting opportunities to collaborate with MAX through its dedicated services, and for the uptake

[13] https://www.hipeac.net/2021/spring-virtual/#/; https://www.hipeac.net/2021/spring-virtual/#/program/.
[14] https://events.prace-ri.eu/event/1018/page/116-pracedays21-call-for-posters.

of its codes within their environments. Targeted engagement channels include podcasts, testimonials, articles in relevant media and press channels, targeting industrial readers based on end-user interviews and across the social media channels.
A premier industry event is already part of the stakeholder engagement plan:

- **36th International CAE Conference and Exhibition**[15] (Virtual Event, 30/11-4/12/2020). Participation in collaboration with FocusCoE and Excellerat, the European Centre of Excellence for engineering application. At this industry event on computational engineering, MAX will have a booth as part of the vExhibition.

Other planned events include:

- **EU Sustainable Energy Week EUSEW 2021**[16], the largest European conference dedicated to renewables and efficient energy use in Europe with a focus on sustainable energy issues, new policy developments and best practices.
- **European Materials Modelling Conference** (March 2021)[17], an event aimed at boosting networking between European and international stakeholders, hosting all main stakeholders in the materials modelling field.
- **International Supercomputing Conference** (ISC; June 2021). Industry participation is an opportunity to draw attention to MAX's support services.

Other events will be sourced through several channels: the event tracker, a continuous scan of the offer; invitations to specific events; on-going collaboration with FocusCoE and CoE stakeholders.

Figure 6: Industry User of MAX - Testimonial Card. An example of a Testimonial Card for an industrial end-user, one of the features for the MAX showcases.

[15] https://www.caeconference.com/.
[16] https://www.eusew.eu/.
[17] https://emmc.eu/.

- **Research and Academia**:

The engagement plan for M25-36 is to ensure regular interactions with this stakeholder group with a view to:

  - Continuing the high-quality dissemination activities of scientific results (publications, talks, posters).
  - Increasing awareness of MAX and opportunities for uptake of the flagship codes and other results.
  - Collecting user testimonials and stories for a well-grounded view of the benefits of MAX. These will be a mix of testimonial cards, user stories, and interviews.
  - Supporting the acquisition of new knowledge through the training programme.
  - Sharing advances through scientific conferences, webinars and other virtual formats to ensure researchers are kept abreast of developments in the field.

Opportunities to engage with this stakeholder group come in the form of several major events. One example is given below.

- **Psi-k Conference 2021**, (23-26 August 2021)[18] participation in the design and organization of the Psi-k-2020 conference (initially planned for September 2020 in Lausanne, now rescheduled to August 2021, due to COVID-19 emergency): specific MaX contributions will include a dedicated booth, the organization/participation/chair in several thematic sessions, a specific MaX event after the conference closure. Psi-k typically involves 1000+ computational scientists in the field of materials science. It is the world's largest event on electronic structure for the international community working on the development of fundamental theory, algorithms and computer codes to understand, predict and design materials properties and functions.

Figure 7: Research and Academia Users of MAX - Testimonial Cards. These cards will be replicated in the updated plan to expand coverage of the end-user perspectives.

[18] https://www.psik2020.net

- **General Public**

The engagement plan for the general public in the period M25-36 is to find new ways to increase awareness about materials science and HPC in its transition towards exascale. ESOF2020 - EuroScience Open Forum (September 2020) was an opportunity to highlight the role of supercomputing in advancing science also to a layman audience. The strategy for continued engagement includes tailored content easily digestible by the public with key insights into what advances mean in everyday terms. MAX will leverage social media channels to convey these key messages to social groups and civil society and will also promote short video-chunks from the webinars and replicate them over time.
These actions suffer the most of the pandemic situation, as it is difficult for the general public to look for events. Therefore channels different from virtual events must be pushed. Nonetheless, the experience in this field include, e.g., the participation in

- **European Researchers' Night 2020**[19] (and editions to come), an EU-wide public event bringing researchers closer to the general public. The event highlights the diversity of science and its impact on citizen's daily lives. It also aims to encourage interest in research careers, especially among young people. In 2019, the event attracted 1.6 million visitors from 400 cities in Europe and beyond. Confirmed participation of MAX is an important opportunity to promote the project to a broader audience.

Other elements of the strategy include creating short 60-second interviews featuring Code Developers to give a lightweight explanation of the key characteristics of each code. These will be guided by templates with straightforward questions to ensure the messaging is clear for outsiders of the MAX project.

2.3 Channels

MAX uses various communication channels, leveraging the project's networks as these expand over time. Communication formats are tailored to the information needs and interests of the diverse stakeholders with relevant calls to action, drawing on the project's extensive knowledge and experience. The main channels utilized in MAX for M25-36 are listed in Table 3 and Table 6, which update the original plan in view of new measures introduced to the communications strategy.

2.3.1 Social Media Channels and Professional Networks

Community-centric channels are an essential part of the communications strategy as they bring MAX into direct contact with stakeholders and enable profiling from a qualitative perspective. Much of their value lies in not being bound by physical interaction, time or place, especially so in times of global pandemics.

[19] https://ec.europa.eu/research/mariecurieactions/news/results-msca-night-2020_en.

These channels also enable MAX to track on-going discussions, developments and interests, become directly involved in conversations, sharing invitations through direct messaging and using visuals to attract attention.
The overall design and promotion of MAX stakeholder engagement, correlated content creation and development, and social media campaigns are coordinated through regular communications from MAX management and other partners to deliver the most accurate, relevant, and updated news and insights through the main social media channels. In MAX the three main channels of communication used to strengthen engagement are: Twitter, LinkedIn, YouTube.

2.3.1.1 Twitter

MAX uses this social networking platform to convey short, snappy messages about its activities. A great use of Twitter cards is done, as they are graphically designed to capture attention to convey a message. Nonetheless, they can be the voice of the consortium as well as of testimonials.
Below the Twitter campaign for the webinar series on the codes is presented, and the pattern for different events is given.

Figure 8: Sample of a SMART Campaign on Twitter.Top: the official Twitter card for the webinar, marking the launch of the campaign. Bottom left: example of the high level of engagement on Twitter (i.e. 12 retweets and 24 likes). Bottom-center & bottom right: various phases of the campaign (pre, during and post event).

Twitter Achievements at M24

Achievements bear testimony to the value of this approach to social campaigns, which will continue in the next project phase:

- 1,136 tweets garnering over 1.69M impressions, 440 mentions, 4.8K likes and 2.1K retweets.
- 46% growth in Twitter followers since May 2019 (D9.1 submission month).

2.3.1.2 LinkedIn

MAX uses this professional network to share regular updates, promote activities, engage with members and expand the community. SMART campaigns follow the same route as on Twitter.
This channel is used to promote the MAX events, such as workshops and webinars, where the latest developments are showcased. SMART campaigns are used here to increase momentum around a MAX activity over a certain timeframe, as shown in the figure below.

Figure 9: Example of a SMART Campaign on LinkedIn. Up: launch of the webinar campaign; Down: zoom in on panellists.

The same approach is used for all MAX activities that have a defined timeline, and usually where there is an action for stakeholders, e.g. register for a webinar, visit an updated or new page on the website.

LinkedIn Achievements at M24

- 207 posts.
- 298 followers.
- 53% increase in the LinkedIn followers since May 2019.

2.3.1.3 YouTube

MAX uses this channel to collect, share and promote its videos, tutorials and webinar recordings that remain always at the public's disposal.

Figure 10: Sample of Webinar Recordings on the MAX YouTube Channel.

YouTube Achievements at M24

- 17 videos (7 recordings and 10 other videos) uploaded on YouTube Channel since the start of the project.
- 1463 views of the webinar recordings (7 recordings uploaded between May and November 2020).
- 3214 total number of video views since the start of the project.

Plans for M25-36 include campaigns to further increase the visibility of YouTube videos, potentially with low-budget advertising campaigns as an effective means to achieve yet higher views.

Summary of Next Steps for MAX Social Media Channels

- Carry out regular SMART campaigns on Twitter and LinkedIn, promoting MAX visibility at events, achievements and impacts, including end-user engagement.
- Engage with stakeholders through the LinkedIn network, including dedicated dialogues of MAX-specific topics with a view to triggering insights and driving uptake potential.
- Upload new webinar recordings as they happen, including training tutorials.
- Create shorter versions of the YouTube webinar videos . The aim is to focus on specific insights and advances to ensure more digestible and easily consumed by stakeholder groups targeted .
- Carry out campaigns to further increase visibility of the YouTube videos, investigating the potential use of small-budget advertising campaigns.
- Continue to track impacts in the KPI assessments across the social media channels.

2.3.2 Events

To maximize impact towards stakeholders and in collaboration with partners, MAX will continue to target relevant events through digital interactions, while waiting to go back to post-pandemia physical events.

2.3.2.1 3rd-party Events

Events targeted span workshops, coordination meetings, scientific conferences, fairs and exhibitions, webinars, training and tutorials organized by 3rd parties dedicated to HPC, HPT and HPDA; materials science and related emerging technologies, as well as CoE coordination activities. Building on successful synergies is another key element of the updated plan, again looking for digital alternatives wherever possible to guarantee continued interaction.

To streamline 3rd-party event selection and partner inputs, a new internal template is being created indicating specific roles MAX could play (e.g. talks, panels, papers, posters) along with stakeholder involved, planned communication activities and expected outcomes. The template also covers aspects

such as co-branded and co-organized events to highlight higher levels of visibility for MAX, as well as paper submissions.

2.3.2.2 MAX Events

These include MAX training events and a final MAX workshop, which will zoom in on the major achievements of MAX. Training events take place through WP8 in close collaboration with the developer teams, ensuring relevant partners are directly involved in stakeholder discussions. A special case is given by the collaboration with Psi-k and CECAM: MAX has agreed to co-fund a series of workshops for broader dissemination and community engagement through these institutions. The main Psi-k conference, that takes place every 5 years planned for 2020 in Lausanne and postponed to 2021, will spot selected joint MAX - Psi-k activities including a scientific session and two community sessions/events especially targeted to young people and women. The same applies to events supported by FocusCoE, other CoEs, new consortia on exascale, and the Graphene Flagship, among others.

The focus, format and agenda of the final MAX workshop will be defined in concert with the consortium partners with targeted stakeholders foremost in mind. A recruitment campaign for the event (physical or virtual tbc) will be defined per stakeholder group with dedicated event announcement banners. The run-up to the event will be complemented by the rollout of a compelling package on the results and impacts of MAX, spanning its main assets and end-user perspectives. Depending on the final format, the event will also feature a series of interviews and interactive sessions.

Further opportunities are constantly monitored throughout the lifecycle of MAX to ensure the project is on stand-by to take part in any relevant events. Flexibility is thus a key measure in place for M25-36, so partners are encouraged to contribute whenever possible and the communications team can move swiftly to promote MAX involvement. Clearly, there are lessons to be learned from the transition from physical to digital and MAX will take these on board in its interactions, moving forward.

2.3.2.3 MAX Webinars

MAX webinars have been a key asset for stakeholder engagement and dissemination and therefore a central element of the plan. The main strategic goals are:

- Ensuring opportunities for training and access to webinar recordings and presentations afterwards.
- Extending outreach to existing and prospective users of MAX products and services with practical how to get started guides.
- Broadcasting the flagship code porting and exascale capabilities for materials science.

- Interacting with a wide pool of stakeholders across the globe while helping to enhance engagement levers for those hard-to-reach segments.
- Having an effective launchpad for new releases.

In 2020, a Webinar Series on Flagship Codes was carried out with a view to effectively feature the activity taking place behind the MAX's codes and to provide the community with valuable information on the actual deployment, usage and characteristics of the codes. The series spanned from May to November 2020 and managed to gather 947 participants coming from 67 different countries worldwide.

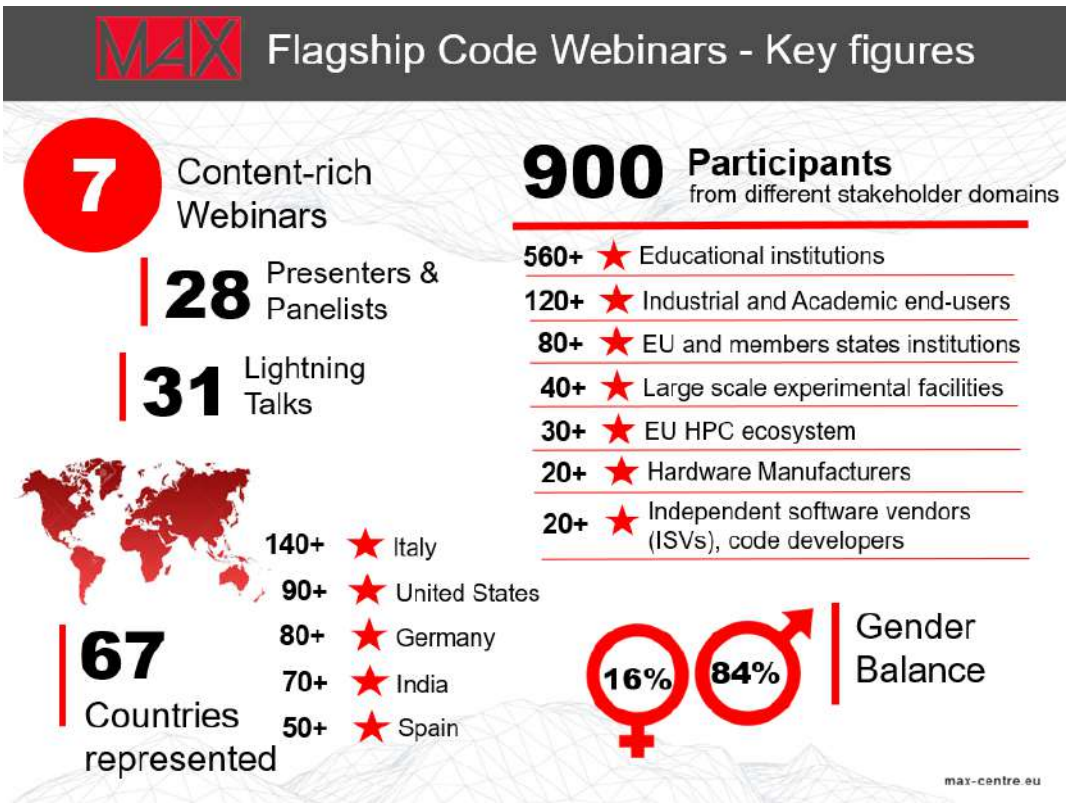


Figure 11: Key figures of MAX Webinar Series on Flagship Codes.

Impacts of the webinars on social media were tracked throughout the campaigns.

SMART Campaign: Flagship code webinars	Partner	Time frame: May 2020 – November 2020	Impacts Achieved: LinkedIn and Twitter
Quantum ESPRESSO	SISSA, CNR, CINECA	13 May 2020	79.6K impressions, 153 likes, 61 shares – TOP TWEET (April 2020)
AiiDA	EPFL	27 May 2020	15.5K impressions, 120 likes, 35 shares TOP TWEET (May 2020)
YAMBO	CNR, CINECA	16 June 2020	16.1K impressions, 122 likes, 44 shares - TWEETS MOST POPULAR MEDIA (June 2020)
CP2K	ETH ZURICH	24 June 2020	23K impressions, 146 likes, 43 shares - TOP TWEET and MOST POPULAR MENTIONS (June 2020)
SIESTA	ICN2	22 September 2020	37K impressions, 209 likes, 81 shares - TOP TWEET and MOST POPULAR MENTIONS (September 2020)
FLEUR	JUELICH	14 October 2020	14K impressions, 93 likes, 25 shares - MOST POPULAR MENTIONS (October 2020)
BigDFT	CEA	12 November 2020	13K impressions, 102 likes, 29 shares - MOST POPULAR TWEETS, MENTIONS (October 2020)

Table 1: SMART Campaign. Outcomes for the Flagship Code Webinar Series.

To properly explain the work done for Flagship Code webinars, and repliable for similar activities to come, we present here as an example of success story the "Yambo code Webinar" event.

The third Webinar of this Flagship Code series put the Yambo code into the spotlight on the 16th of June 2020 with the title "*Quasiparticle Band Structures and Excitons in Novel Materials using the Yambo Code*".

The Webinar featured the researchers that are currently involved in the development of Yambo and offered the following main takeaways to the participants:

- An exhaustive overview of the Yambo code.
- A timely update of the status of the GPU version and outline of roadmap for its future evolution.
- A basic set of instructions on how to tune and use the code efficiently on new HPC systems.

Figure 12: Branded campaign specifically devised for the Yambo Webinar.

The Webinar turned out to be a very successful event with a collective audience of 185 attendees (out of 247 registrants) from widespread scientific and technological background and coming from 44 countries (21 of which were EU member states). A success that is also mirrored by the significantly high degree of engagement of the audience, resulted in 97 direct questions to the speakers.

The Webinar underwent a thorough work plan of promotional, outreach and dissemination activities spanning through the pre- and post-event, following the modus operandi envisaged for each Webinar.

- Creation of standardised and branded graphics
- Set-up of a dedicated registration page on the MAX website
- Tailored Email campaign to reach out the entire network of Stakeholders
- Social Media regular activity
- Live Tweeting during the event
- Upload and release of the recorded Webinar and speaker presentations
- Post-event "Thank You message" addressing the participants
- Satisfaction Survey on the event
- Repurpose the content on Social Media in the following weeks

2.3.2.4 Podcasts

Podcasts as a communications medium are fast becoming mainstream. According to Forbes, there are now 62 million Americans listening to podcasts each week, up from 19 million in 2013[20]. Reasons for this trend include: Growth in the number of podcast choices and low cost entry. Podcasts are also very well suited to making concepts accessible to newcomers and laypeople. The more relaxed and informal format likens them to fireside chats, albeit in virtual format. Podcasts also have the advantage of being able to extract very short extracts ("soundbites") from the recording and sharing them in bite-sized pieces across social media. Twitter banners can also be produced to share key takeaways. Overall, podcasts are a means to entice new listeners and engage them in interesting conversations.

The updated plan therefore foresees the use of podcasts availing from first-hand experience, dedicated editorial software and platforms for making the podcasts publicly available. The organization of podcasts will entail:

- Defining the podcast theme, title and timeline (from preparation to post-production and promotion).
- Creating a straightforward storyboard with questions for the selected guests (up to 3).
- Organizing a practice session to prepare guests.
- Recording the podcast and time-stamping the storyboard.
- Putting together the full recording and selected extracts and uploading all on the dedicated platform.
- Checking guests' satisfaction.
- Carrying out the promotional campaign after making the podcast live.

The plan foresees up to four podcasts in the period M25-36. They are expected to target the following topics and stakeholders:

- Beginner's Guide to Materials Science and advanced HPC capabilities. General public and young researchers setting out on their careers.
- An Insider's Look at the flagship codes with 1-2 examples. Academia and research; industry.
- User insights into MAX, highlighting tangible benefits and takeaways. Academia and research; industry.
- A Dive into the journey towards exascale. This could potentially target all four priority stakeholders.

2.3.3 Broadcasting outcomes of events

MAX divulges the main outcomes through its social media and networks, highlighting advances and progress towards exascale, user benefits, utilizing SMART approach as defined in Section 2.3.7 below.

[20] https://www.forbes.com/sites/bradadgate/2019/11/18/podcasting-is-going-mainstream/?sh=348dd9021699.

Each promotional campaign is geared towards specific stakeholders, whether that be educational institutions, academia and research, or industry. On-going discussions help share past experiences and lessons learnt in terms of reaching out to industry players, conveying value propositions and coordinating activities.

2.3.4 Scientific Publications

Scientific publications are a strategic means of dissemination for most of the Consortium partners. They intend to keep their effort in sharing acquired knowledge on codes and also to increase visibility of HPC, HPT and HPDA as emerging core advancements.
Data for publications up to M24 are summarized below.

- 32 research papers published so far in 2020
- 16 research papers published in 2019
- 1 research papers published in 2018
- 3 submitted papers (submission version or pre-print version available at this stage)

Total: 52 research papers, 48 already published, the large majority (45) are compliant with Open Access rules. For the complete list see Annex 2 at the end of this document.

Figure 13: Samples of recent Scientific Publications.

For more details on all MAX scientific publications, see Annex 2 - List of MaX Scientific Publications.

2.3.5 Traditional Media and Other Channels

MAX will also target popular channels for research results and advances, including specialised channels on HPC and channels covering materials sciences. Its aim is to broadcast results to a more diverse set of stakeholders, including the wider research community, policy makers and citizens.

To this end, a new series of announcements along the theme of "*Spotlight on MAX Advances*" will be published on the MAX website with a dedicated banner to visually distinguish the news items. Press releases on major announcements are also foreseen.

In both cases, new items will also be promoted via the social media channels.

Dissemination Channel/Venue	Channel Type and Geographical Coverage	Main Purpose and Targeted stakeholders
CORDIS[21] @CORDIS_EU	EC's primary source of results from funded projects, publishing research results to professionals in the field to foster open science and innovation.	Promote MAX events and broadcast advances and achievements to general audiences. Submissions for the "Results Pack" and of press releases.
EuroHPC[22] @EuroHPC_JU	Joint Undertaking on HPC in Europe.	Submit news items on important announcements on MAX. Press releases.
HPCWire[23]	News and information resource covering HPC trends and technologies and analysis.	Create tailored articles on MAX advances and benefits for end-users. Press releases.
Inside HPC[24]	Blog on news and events in the world of HPC conveyed in bite-sized nuggets as a resource for supercomputing professionals.	Create tailored articles on MAX advances and benefits for end-users. Press releases.
Primeur Magazine[25] @primeurmagazine	Europe's only independent digital magazine focusing on High-Performance Computing (HPC).	Create tailored articles and other formats that convey complex research and technology in more digestible languages. Press releases.
Supercomputing Online[26] @SC_Online	International magazine on the evolving landscape and its unique benefits.	Create tailored articles on MAX advances for professionals in the field, including press releases.

Table 2: Sample of targeted media channels.

[21] https://cordis.europa.eu/.
[22] https://eurohpc-ju.europa.eu/.
[23] https://www.hpcwire.com/.
[24] https://insidehpc.com/.
[25] http://primeurmagazine.com/.
[26] https://www.supercomputingonline.com/.

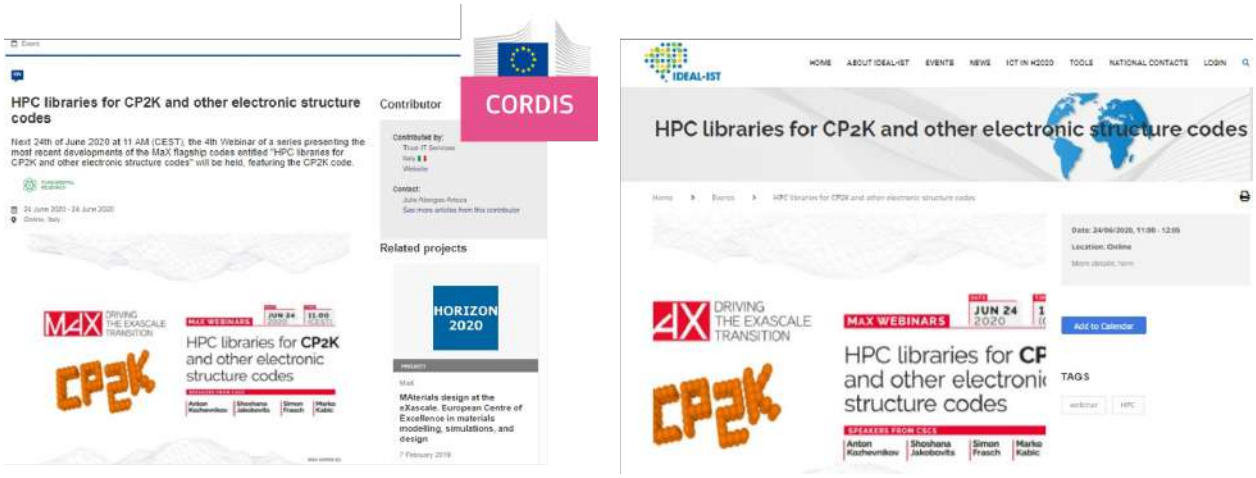


Figure 14: Sample of Articles and Announcements on external Media Channels.

Summary of Next Steps for scientific publications and articles in research and HPC channels

- Create a new series of articles: *Spotlight on MAX Advances* with dedicated banners and visuals.
- Work with partners to track submissions to scientific journals and new publications, using the dedicated template from MAX management.
- Broadcast the publications more widely across social media and the professional network, highlighting the main advances.
- Feature the publications in future newsletters.

2.3.6 MAX Service-oriented Web Platform

The website (http://max-centre.eu/) acts as the key-channel for communication and engagement for the whole MAX's community.

Rebuilt from the previous Wordpress MaX website, the new revamped version is based on Drupal and was launched in October 2019. The website underwent multiple iterations that have been carried out with a view to improve both the main functionalities and the overall outer layout.

The Graphic Design aspect plays a fundamental part of the website in the pursuit of relevant objectives:

- Ensure a pleasant UX (User Experience) by increasing its visual appeal, sense of professionalism, usability and brand value.
- Provide harmonised branding that also reflects across the external digital channels.
- Facilitate the navigational steps of the users through a clear section's breakdown and tailored icons to diversify (and define) the different websites areas.

On top of this, the website serves as a timely and constantly updated **repository of trustworthy sources of information for the relative materials science and HPC communities:** an easily accessible gateway where each section aims at responding at specific requests of the users.

Here under the most notable features and updates that contributed to make the web platform more comprehensive, usable and helpful for the MAX community:

- **About MAX –** This section serves the purpose to provide a clearer and easier understanding of the overall project, aimed at achieving a deeper involvement of the general public (*i.e* the "MAX *in a nutshell*" area). Among others a "*News & Events"* section perfectly displays the features of events, a, e.g., concretely upholds the outreach of the activities carried out within WP8.
- **Services –** A section focused on the delivery of a competent and prompt user support and consulting services to serve the community of Research, Academia and Industry.
- **Training** – This area offers a wide range of freely accessible educational material produced by WP8 in the HPC and materials science domain for each flagship code, spanning from online courses and schools, lectures, workshops and webinars with a view to contribute to fill the sectoral skills gap.
- **Facts and Figures** – Some of the main sections (*Data, Services and Training*) have been upgraded with a personalized *"Facts & Figures"* space to provide a concise view of the main outputs and achievements through visual infographics.
- **Frequently Asked Questions** – An overarching FAQs section has been implemented to facilitate the research of answers to the most common issues linked to the flagship codes as well as the possibility to sift straight through the FAQs page of every HPC centre of the consortium.

Summary of achievements at M24

01 January 2020 – 25 October 2020

Users	Sessions	Avg. Session Duration	Pageviews	Avg. Time on Page
18.739,0	25.660,0	00:01:51	51.758	00:01:49

01 January 2019 – 25 October 2019

Users	Sessions	Avg. Session Duration	Pageviews	Avg. Time on Page
10.331,0	14.840,0	00:01:29	25.390	00:02:04

Figure 15: Website Achievements at M24 with YoY Growth: all the primary analytics almost doubled in 2020 compared to 2019 (Year-to-Year analysis).

Summary of Next Steps for the MAX website

- Continue to track impacts of the website through the dedicated dashboard.
- Ensure a content-rich and user-centric approach to populate the website.
- Implement a Science@MAX section to demonstrate how the MAX flagship codes can enable the achievement of scientific results for other research centres or groups.
- Showcase on the website the community engagement, possibly with a section designed to feature end-users or stakeholders benefiting from the usage of codes.
- Feature updates from the in future newsletters, as relevant.

2.3.7 SMART Campaigns

The strategy for MAX promotional campaigns implements the SMART approach:

- **Specific**: Having a clear objective, e.g. promote a MAX webinar, its opportunities for the community and hands-on approach.
- **Measurable**: Tracking quantitative impacts, e.g. number of views on social media, professional networks and visibility on 3rd-party channels; number of webinar participants recruited.
- **Actionable**: Having a specific end-goal, e.g. recruiting new community members, driving uptake of MAX codes, services, divulging training opportunities etc.
- **Relevant**: Creating tailored messages for the stakeholders targeted.
- **Time-bound**: Setting clear start and end dates, e.g. from the launch of the webinar campaign, to the monitoring of results achieved (measurable) and end of the campaign with the publication of the insights, recording and presentations.

Such an approach enables MAX to define a clear set of objectives for each campaign as essential elements for achieving impacts, from both a quantitative and qualitative perspective. They are therefore a key element of the communications strategy and can be applied to activities like MAX events, training, new insights and advances, press releases, 3rd-party events. They are also a very practical way of updating related KPIs.

As they are time-bound, they are typically carried out prior, during, and after a specific campaign to act as teasers, increase visibility of MAX, and highlight the main takeaways and impacts.

2.3.8 KPI-driven Approach and Communication Toolbox

The MAX strategy for communication, dissemination and stakeholder engagement is underpinned by a KPI-driven approach for the entire duration of the project. Impacts are tracked continuously and a customized dashboard is used for a core set of targets.

The plan defines a set of macro activities, detailing more specific activities through a live editorial plan aimed at ensuring an all-partner inputs based on effort allocated to maximize impacts not only in terms of outreach but also uptake of MAX. Impacts are tracked through a customized screenshot, with examples given in Section 5.

Monthly "Flash Reports" track the latest updates on visibility, engagement, community development and dissemination, keeping the consortium abreast of progress and showing them the impacts of joint efforts. These monthly Flash Reports cover:

- Community growth: data collected monthly through the customized Dashboard plus the newly recruited members of the community profiled in the database.
- Website impacts: data collected monthly through the customized Dashboard.
- Stakeholder engagement: outcomes of recent past events and upcoming events.
- Updates on scientific publications (recently submitted or published).
- Upcoming events and activities planned for the following period.

As indicated in D9.1, this plan updates KPI-driven activities for the period M24-36,having reported on major impacts up to M18 in D9.2.

A professional and dynamically evolving Communication Toolkit guides the implementation of the plan. The toolkit covers key elements for a content-rich approach tailored to the diverse MAX stakeholders, spanning a variety of formats and channels to reach them. It also supports community building through events, social media and professional networks and supporting training as key to imparting new knowledge among the next generation of HPC specialists and material scientists. Elements include news articles, collaterals and promotional material, videos, webinar recordings, training materials, presentations, press releases and announcements, among others.

Each element is mapped to an activity and a KPI and/or metric acting as a compass for MAX partners.

The table below updates the toolkit elements and targets for the period M25-36.

Activity Focus	Toolkit element	KPI Targets for M25-36
Website content population, including content tailored to 4 priority groups	News pieces on website	1/week; 250 unique visitors; 400 page views 1 tailored content/quarter
Communications	Press releases	min 1 press release or article/year for specialist press.

	Graphically designed material (Flyers, posters, pop-up banners, infographics, brochures etc. tailored to different stakeholders and regularly updated to reflect project progress	Min. 1 updated project flier M25-36 Min. 1 booklet on assets. Min. 1 booklet on end-user stories Min. 1 Final Impact Report
	Webinar recordings and Training material available online	List of training resources, including links to YouTube Channel (Workshops and Schools) Presentations from webinars Updated Project Slidedeck
	Newsletters	1 every 3 months
Digital community interaction	Twitter, including SMART promotional campaigns	Min. 3 Tweets/week Multiple Tweets for promotional campaigns and events. KPI: increase female followers from 26% to 35%.
	LinkedIn, including SMART promotional campaigns	Min. 1 post/week
	YouTube	Min. 1 project video/year for newcomers. Min. 3 training-related videos
Stakeholder engagement: 3rd-party events (physical/virtual)	Conferences, workshops, summits	5-10 min. in M25-36 (close monitoring of event

		opportunities and roles for MAX)
Virtual Stakeholder engagement	webinars and podcasts	Min 2 webinars Min 2 podcasts
Articles targeting professionals and researchers in the field	Features on advances and achievements	Min 2 articles in online channel (results, advances in HPC and/or materials science)

Table 3: Updated Communications Toolkit.

3. MAX Results and Assets for Dissemination & Communication

MAX is a pan-European central hub for developers and users of materials science leveraging advanced HPC capabilities, driving and enhancing Europe's leadership in the field. The European flagship codes are strategically positioned for advances stemming from pre-exascale, and ultimately transition towards exascale. It supports the continuous co-design activities needed to adapt to upcoming architectures.
It supports efforts to ensure strategic know-how on HPC infrastructure and federates the ecosystem in the materials science domain critical for competitive advantage.
MAX directly addresses one of the main challenges faced by scientific code groups:

- The successful deployment and evolution of the most widely used open-source, community codes, on the pre-exascale machines expected by the end of the project, and to prepare them for the transition to exascale;
- To remove the barriers that prevent them from offering their services and training to the research market, developers, end users and the general public in adopting the current codes to the commercial services.

3.1 Flagship Codes

Information and details on the flagship codes and forums are accessible at http://max-centre.eu/codes-max and http://max-centre.eu/software/product/codes.
The overarching goal of the M25-36 plan is to put greater emphasis on practical aspects and support available to the end-user community. To this end, a user-centric approach is being adopted, highlighting the benefits and the support available. Drawing and building on the highly successful

webinar series, the plan integrates user needs collected through these events with a view to fostering further uptake. Actions foreseen include end-user Testimonial cards for social media, as well as more detailed user stories that can be promoted individually and collectively as one of the major success stories delivered by MAX.

Name & Main MAX Developers	Added value of the Code	License	Value Proposition/Practical guides and support for Users
QUANTUM ESPRESSO (QE) SISSA, CNR, CIN	Collection of open-source codes for electronic structure computations widely used for materials research.	GNU-GPL	MAX updates on GPU version of Quantum ESPRESSO and the roadmap for its future evolution. Practical guides on optimal usage on heterogeneous HPC systems and on how to compile and tune up Quantum ESPRESSO for GPUs, and which tools and libraries are needed. Best practices, tips and tricks of QE on Marconi100.
SIESTA ICN2, BSC	SIESTA has enabled the treatment of large systems with first-principles electronic structure methods for over two decades bringing new opportunities to many disciplines.	GNU-GPL	Guides on preparing materials-simulation codes for upcoming extreme-scale HPC systems. Keeping community abreast of key developments for HPC and scalability; integration of solver libraries; TranSIESTA module for transport simulations. User support for MAX and SIESTA communities.
YAMBO CNR	An open-source project aimed at studying excited state properties of condensed matter systems from first principles using many-	GNU-GPL	Guides on Yambo, where to get it from; how to use and finetune it; how to use it efficiently on new HPC systems. Updates on status of GPU version and future evolution roadmap. New features of the code in real-time

	body methods).		simulations beyond nonlinear optical spectroscopy.
FLEUR JUELICH	Open-source code FLEUR code that provides reference results, utilized to study details of the electronic, magnetic, and atomistic structure of complex materials.	MIT	Guides on features and fundamentals of FLEUR. Updates on functionalities and use of FLAPW method; applicability on large magnetic setup. Insights into possible future applications.
CP2K CSCS	A quantum chemistry and solid state physics software package that can perform atomistic simulations of solid state, liquid, molecular, periodic, material, crystal, and biological systems.	GNU-GPL	Insights on HPC problems arising from large-scale electronic structure calculations with localized basis. Guide on HPC libraries in accelerating electronic structure code. Opportunities to collaborate with developers of HPC libraries within the MAX flagship code.
BIGDFT CEA	An electronic structure pseudopotential code that employs Daubechies wavelets as a computational basis, designed for usage on massively parallel architectures.	GNU-GPL	Insights on basic features, peculiarities and formalism of BigDFT and possible future developments. Guide on theoretical background and fields of application.

AiiDA Platform EPFL	A tool for workflow management and provenance tracking backed by a significant community of users and developers and with interfaces to over 30 materials science codes. AiiDA's permissive open source license (MIT) enables participants to use it both in academic and commercial settings. Its general design and flexible plugin system mean that AiiDA is easily extended to new codes and new use cases.	MIT	Insights into how AiiDA supports users in managing their computational workflows and generated data. Guide on how the AiiDA code can be used to automate workflows that directly use the other MAX flagship codes, e.g. QE. Guides on how the AiiDA lab provides a user-friendly GUI to the workflows, also for non-experts. Guides on how the resulting data can easily be published through the Materials Cloud Archive.

Table 4: Overview of Flagship Codes, drawing on updates conveyed in close synergy with the consortium.

Summary of Next Steps for the MAX Flagship Codes

- Broadcast the impacts and insights from the webinar series.
- Produce a graphically designed Impact Report.
- Carry out a SMART campaign highlighting the main takeaways from the Report.
- Continue collecting end-user testimonials for the creation of Testimonials cards and user stories (based on a straightforward template).
- Explore opportunities to present the codes and their users in MAX and 3rd-party events.
- Include the impacts in the final results package for MAX.

3.2 MAX Products and Services

The following **products** are available on the MAX website where all the information is readily accessible and reusable by all stakeholders, especially those groups helping to increase adoption:

- **Features and applications**: http://max-centre.eu/product/features-and-algorithms.

- QE, Yambo, Siesta, Fleur

- **Software Libraries**: http://max-centre.eu/product/libraries that are specific to the materials modelling domain. The libraries contain functions that perform basic quantum chemistry materials science operations or systems and mathematical tasks.
- **Workflow**: http://max-centre.eu/product/workflows. AiiDA high-throughput environment supporting simulation codes via plugins is presented.

The following **services** are publicly available on the MAX website:

- **Helpdesk**: http://max-centre.eu/service/max-help-desk. Basic support and assistance in the domain of materials science.
- **High-level consultancy**: http://max-centre.eu/service/max-high-level-consultancy. High level support service for MAX users enabling them to exploit software tools in the materials domain.
- **Simulations on premise and in the cloud**: http://max-centre.eu/service/simulations-premises-and-cloud. AiiDA lab, a cloud platform for accessible Materials Simulations; Quantum Mobile— a VirtualBox machine that comes with AiiDA and a set of commonly used quantum codes preinstalled.
- **Turnkey materials solutions**: http://max-centre.eu/service/turn-key-materials-solutions. Solutions for the automatic computation of advanced materials properties leveraging AiiDA and workflows for the MAX flagship codes.
- **Services to the industry**: http://max-centre.eu/services-industry. Personalised consultancy to industries for specific and targeted needs.

Summary of Next Steps for MAX Products and Services

- Trigger web page updates from relevant consortium partners and the necessary timeframe.
- Co-define the overall value proposition for the target audience(s) as part of the larger campaign on MAX assets.
- Create campaign banners with key takeaway and stakeholder call to action.
- Carry out the campaign and monitor outcomes.
- Collect all relevant information for a dedicated booklet to be graphically designed towards the end of the project.

3.3 Materials Cloud Platform

The MAX Materials Cloud is an Open Science Platform designed to enable the seamless sharing of resources in computational materials science. The platform is designed to enable the open and seamless sharing of resources for computational science, driven by applications in materials modelling. The platform hosts:

- Archival and dissemination services for raw and curated data, together with their provenance graph.

- Modelling services and virtual machines.
- Tools for data analytics.
- Pre-/post-processing.
- Educational materials.

Data is citable and archived persistently, with comprehensive coverage of entire simulation pipelines (calculations performed, codes used, data generated) in the form of graphs that allow retracing and reproducing any computed result. When an AiiDA database is shared on Materials Cloud, peers can browse the interconnected record of simulations, download individual files or the full database, and start their research from the results of the original authors. The infrastructure is agnostic to the specific simulation codes used and can support diverse applications in computational science that transcend its initial materials domain.

Summary of Next Steps for MAX Materials Cloud Platform

- Create a set of core messages on the platform in concert with relevant consortium partners aimed at highlighting the value proposition for this MAX asset.
- Create campaign banners with key takeaway and stakeholder call to action.
- Carry out the campaign and monitor outcomes.
- Collect all relevant information for a dedicated booklet to be graphically designed towards the end of the project.

3.4 Exascale

MAX is tackling the challenges of porting, scaling, and optimizing materials science application codes for the peta- and exascale platforms to deliver best code performance and improve users productivity on the upcoming architectures.

Scientific Challenge: Porting, scaling and optimising materials science, open source codes for upcoming exascale architectures.
Strategy: MAX pursues a pragmatic approach based on building knowledge about exascale-related problems and running proof-of-concept co-design and test-field solutions. The resulting best practices are then consolidated in the official (publicly available) code releases.
Outcome: New code versions with validated developments; publicly available libraries and modules; extensive dissemination activities.
Impact: Best exploitation of present and future HPC systems; valuable knowledge for other applications and domains, as well as technology providers.

Summary of Next Steps for communicating the transition to exascale

- Create a set of core messages on how MAX is enabling the transition to exascale:
- Highlighting the value proposition for the materials science community.
- Explaining the transition in layman's terms.
- Create campaign banners with key takeaway tailored to diverse stakeholders.
- Carry out the campaign and monitor outcomes.
- Collect all relevant information for a dedicated booklet to be graphically designed towards the end of the project.

3.5 Training and related Materials

The training activity is one of the most important for MAX, as from Action 4 in the DoA (Widening the access to codes and fostering transfer of know-how to user communities.) and relevant objectives, and is being addressed by WP8. For a full success, it requires a streamlined communication between WP8 and WP9, as events of the training plan need the communication and advert campaigns that so far ensured a high participation and enrollment. This factor also responds to the creation of a solid linkage between WPs activities.

Training and Educational activities represented a key-instrument to support the uptake of MAX Flagship Codes in the first half of the project, especially towards researchers, code users and student/developers.
Before the Covid-19 outbreak and its following side-effects, the spectrum of the Training offering featured a mix of different format spanning from Hackathons, Hands-On schools and Workshops, in-person visits at MAX laboratories, in order to ensure possibility to join to the widest audience of people. While a more detailed list of individual activities can be found in the deliverable 8.2, this is a short sum-up of the main figures:

- 1,500+ Participants (aggregate with Webinars until November 2020).
- 3 schools with hands-on sessions dedicated to the flagship codes (125 students).
- 5 Hackathons and workshops aimed at training code developers (142 participants).
- Participation in schools organised by other parties (11 MAX expert members participated as trainers for more than 310 students).
- Contributions to 4 Master programmes (higher education) with introductory courses on computational materials science, hands-on sessions on usage of MAX flagship codes.
- 38 researchers hosted at MAX laboratories for basic and specialized training on MAX codes and libraries.

Next Steps

Following the Covid-19 consequences, the overall Training and Workshop schedule is undergoing a significant change. Since most of the events are expected to take place on a remote basis at least for the first half of 2021, the plan promptly shifted towards an online format, through the organisation and delivery of tailored online workshops per each of the Flagship Codes with specific focus sessions on the usage of certain parts of the Code.
This is the current calendar, including already postponed and in-progress events:

- Introduction to Aiida, December 2, 2020
- First-principles simulations of materials with SIESTA, February 2021
- All-electron DFT with Fleur - A Hands-on Tutorial, April 12-16, 2021
- Advanced School on Quantum Transport with SIESTA, May 17-21, 2021
- Virtual school on electronic excitations in solids and nanostructures using the Yambo code, Spring 2021
- MAX school on Advanced Materials and Molecular Modelling with Quantum ESPRESSO, Spring 2021
- Introduction to running reproducible workflows with AiiDA, 6-9 July 2021

In this context, it is becoming fundamental to strengthen the participative aspect of each event with a view to enhance the interaction and engagement of participants to the highest level. Talking about the best practices that will be adopted, new online tools will be adopted and optimized to guarantee adequate flexibility and reproduce to the maximum extent the context of physical events (i.e., lectures, parallel Breakout rooms and virtual MeetUps with the Zoom platform; Poster Sessions with GatherTown software). In addition, whenever possible, the sessions of the schools will be spread in few but effective hours for more days, in order to keep high the focus and the participation of the users.

Summary of Next Steps for MAX Training

- Highlight the benefits of training to relevant stakeholders, tailored to their specific needs.
- Carry out recruitment campaigns with dedicated banners.
- Promote the outcomes of the training events with links to resources available, including any tutorials uploaded on YouTube.
- Collect and broadcast trainee benefits through dedicated testimonial cards.
- Conduct short interviews with trainers on a series of training success stories.

4. Communication and Dissemination Plan

4.1 MAX Community

MAX has so far succeeded in building a substantial community with 3420 members. The new interactive features on the website and the highly successful code webinars series have brought more opportunities for stakeholder engagement with key achievements being:

- A community of 3420 members:
  - 2051 profiled members.
  - 959 Twitter followers.
  - 297 LinkedIn members.
  - 113 YouTube subscribers.
- A total of 1,300 webinar registrants and 947 attendees from 67 countries from across the globe, with the largest number of participants from Italy (16%), followed by India and the United States (10%), Germany (9%) and Switzerland (6%).

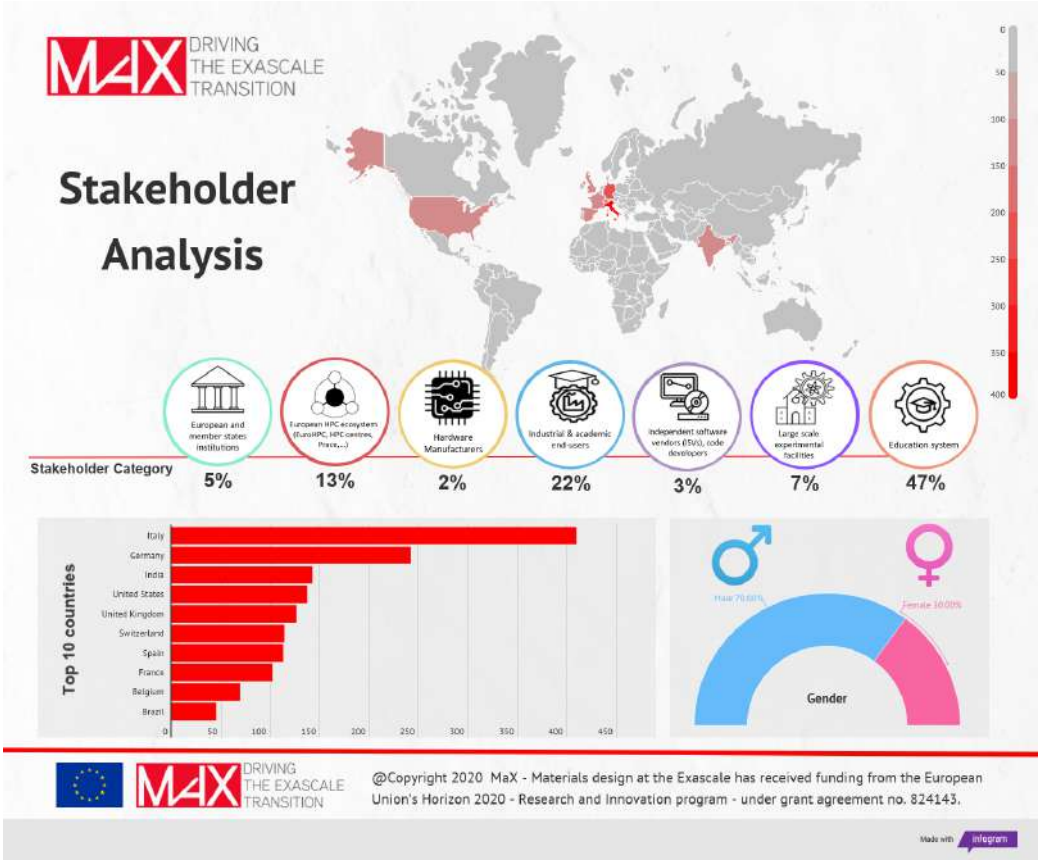


Figure 16: Stakeholder Analysis at M24.Breakdown by stakeholder type and country distribution.

Members of the community are recorded and profiled in a database, which is kept regularly updated to enable MAX to:

- Quantify and qualify its community.
- Tailor communications to diverse MAX types of stakeholders based on the profiling.
- Build better relationships and pinpoint the most active members with whom more targeted interactions can take place.

- Provide better contact response and feedback and elicit responses from the wider public.
- Increase visibility of MAX activities and events.
- Ensure promotional campaigns are successful.

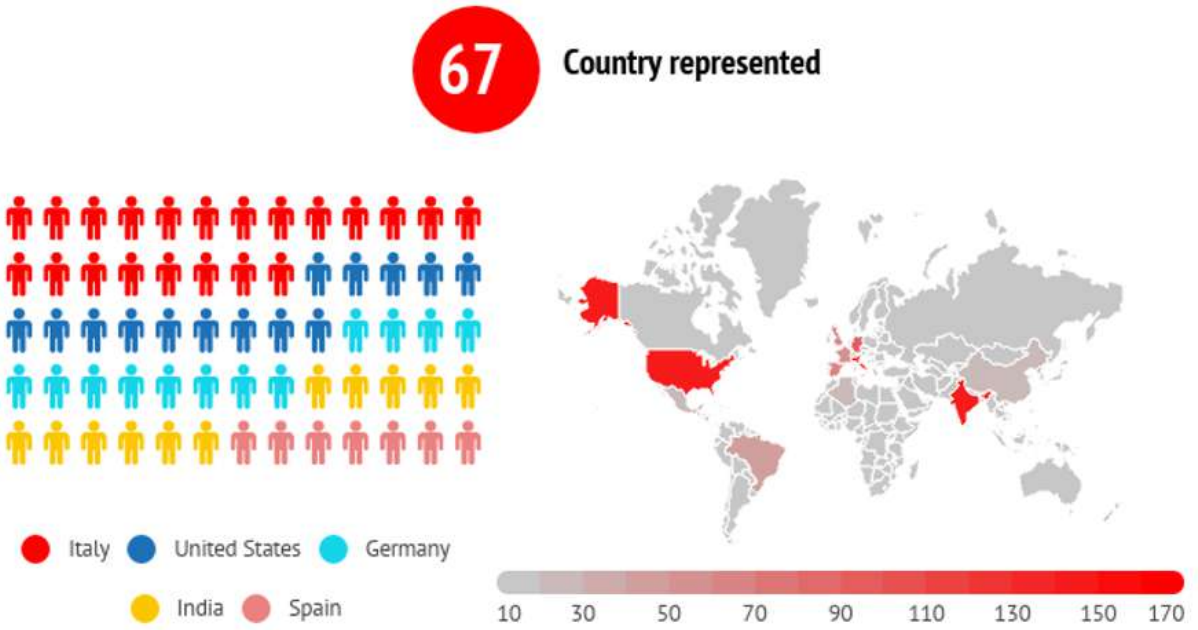


Figure 17: Geographical distribution of MAX webinar attendees.

Summary of next steps

- Create a content-rich and user-centric approach to entice the interest of the community.
- Build relevant synergies with other communities.
- Send personalized invitations to community members for the upcoming events and activities.
- Connect with the MAX end-users and feature them through a series of testimonials cards (to be displayed also on social media) and user stories.

4.2 Content-driven approach

Content is tailored to the specific needs of each stakeholder group, from newcomers to HPC and citizens to long-standing experts in HPC and materials science from industry and research. A wide range of formats will be used to engage stakeholders.

Examples of the content-rich approach include:

- Creating event announcements, e.g. workshops, webinars and training, as part of the SMART-based promotional campaigns.

- Publishing post-events recordings and presentations as a key asset for broadcasting MAX advances available on-demand any time anywhere to stakeholders globally.
- Sharing participant viewpoints as part of the takeaways from the live polling during the events. These also offer key insights on the adoption of the flagship codes as part of the project's user-centric approach.
- Highlighting insights from MAX in strategically important event roles, e.g. select panellists at 3rd-party events, as well as outcomes of 3rd-party events with various roles, e.g. exhibitors, presenters, trainers and tutors.
- Producing user-centric communications material highlighting the benefits of MAX from first-hand experience, including end-users from academia, research and industry.
- Broadcasting advances through papers published in journals, as well as scientific, research and domain-focused channels that target professionals in the field such as e.g. CORDIS.eu.

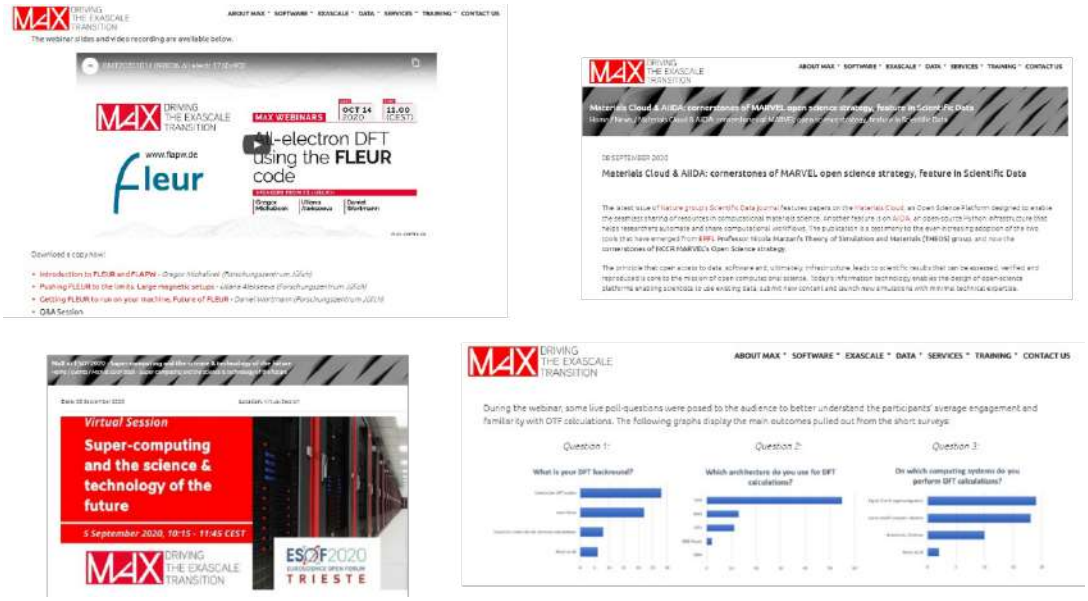


Figure 18: Sample of the MAX Content-rich approach. From top left to bottom right: Webinar recording and presentations; MAX featured in Nature; MAX panellist at ESOF 2020 and poll takeaways from webinars.

The human-centric approach to SMART campaigns through the creation of Testimonial Cards on the uptake of the MAX flagship codes has generated 171.2K impressions on Twitter and LinkedIn and top tweets from April to November, proving the effectiveness of the campaign. This is just the beginning of a series of campaigns targeting end-users aimed at recruiting more adopters of MAX moving forward.

4.2.1 Lessons learnt

- The promotional process now involves preliminary interaction with the project partners to coordinate actions, effort and resources in order to boost visibility and outreach through their digital channels and social media.
- More effort is spent on encouraging external support of MAX's activities and advances through the consolidated synergies and the community at large. One example of this is FocusCoE and its continuous support of MAX's communication activities. Webinar promotion has particularly benefited from this approach with large-scale, personalized campaigns targeting the community of stakeholders.
- Building on the momentum gained through the virtual events by pulling out significant live-takeaways during the event itself. In the case of webinars, this has become the series on Highlights and Insights with content-rich web pages for further messages to the community through social media.
- Strategic tagging of partners and organizations closely related to the news/updates released to max out exposure (thereby avoiding random tags).
- Broadcast news related to the European HPC landscape of which MAX is part to increase awareness of advances in the field as a strategic action for Europe.

Summary of next steps

- Create a brand new story, giving more voice to the end-users or stakeholders that benefit from MAX codes and other advancements.
- Show how the different WPs provide support to each other in the content descriptions with subsequent results.
- Leverage on user-generated content to promote different MAX assets and services.
- Use relevant hashtags and perform aimed hashtag-research to improve brand visibility and find out potential mentions.

4.3 Visual Identity and Branding

A coordinated Visual Identity to benchmark the project was developed out in the first part of the project (see D9.1). Following the development of the web platform with the integration of additional areas and the renaming of some sections, new images have been created to better identify new services and website's units.

The Visual Identity elements and style are seamlessly mirrored throughout all the Communication's items that have been used with outreach purposes (mainly stored within the "***Communication***" section of the website), as the following ones:

- Flyers
- Postcards
- Roll-Up Banners

- Poster(s)
- Graphic Material for events/webinars

Newsletter Branding Enhancements

One example of branding enhancement is offered by the design of the MAX newsletters, which also adopt the content-rich approach. The newsletters have the purpose of keeping MAX community updated on the latest developments, events and activities carried out within the project. The new design and branding of the newsletter have been personalized to make it more user friendly and enticing for readers. The first newsletter of this second edition was issued IN April 2020[27]. It was distributed to a database of 800+ individuals who signed up to receive newsletters AND gained a 41.5% open rate (285 readers) and a total of 153 clicks.

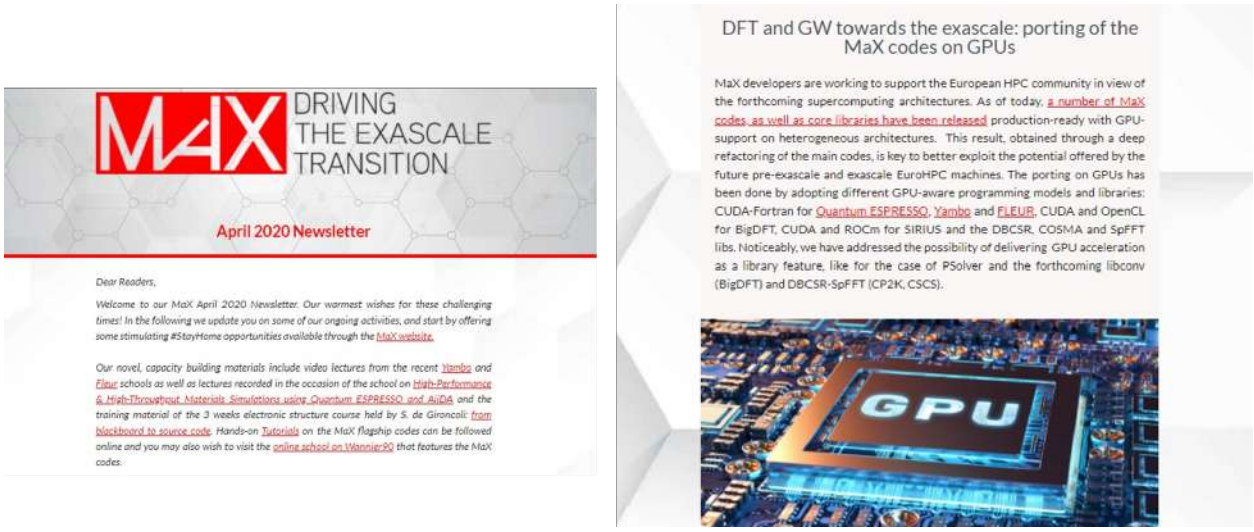


Figure 19: MAX Newsletter.

4.4 Planning Visibility at Events

The main activities aimed at ensuring high visibility of MAX at 3rd-party events include:

- Announcements on the MAX and across its social media channels with relevant hashtags and handles.
- Use of promotional banners.
- Live social media campaigns throughout the event.
- Highlights published on social media and the project website.

[27] https://mailchi.mp/0eb89471350e/max-newsletter-pushing-forward-on-codes-at-the-exascale-and-more-in-2020.

- Tracking of impacts, e.g. visibility (overall and through external channels), number of Tweets, retweets and, where relevant, examples of top media Tweets.

This roadmap is followed also for vExhibition, as this type of event may become more common in the future, and the communication actions undertaken will serve as a pattern for all events to come. The first of such MAX experiences is the CAE Conference and Exhibition (30/11-4/12/2020) accessible through a virtual environment as illustrated in the figure below, which MaX will attend with FocusCoE and Excellerat CoE. Interactions take place remotely, and MAX will have 1-to-1 slots with interested visitors. These will be able to virtually view the materials and links shared on the booth. Data will be collected on the type of visitors going to the stand.

The visibility plan comprises:

- Exhibition page visibility with the MAX logo[28].
- Social media campaign on Twitter and LinkedIn.
- Access to the general MAX flyer, which proves to be equally effective for this type of event during and after the event.

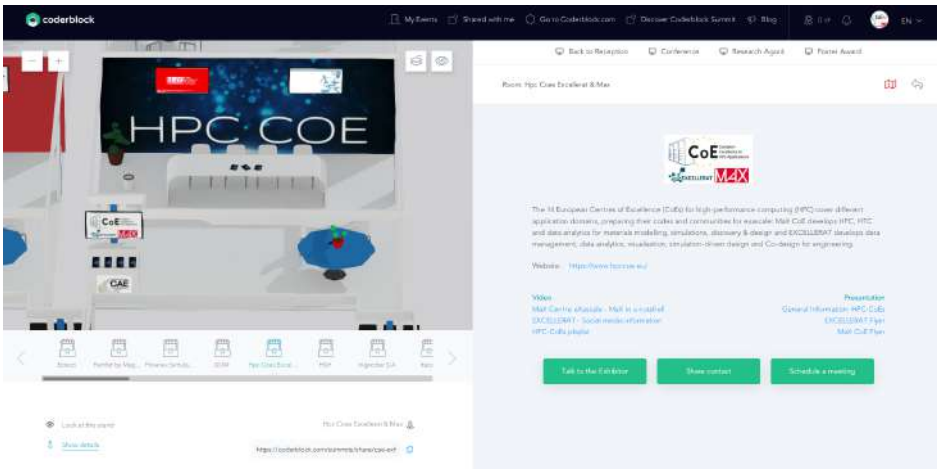


Figure 20: CAE 2020 virtual environment (www.caeconference.com).

4.4.1 3rd-party events in the MAX Calendar

A summary of planned upcoming events is given. It is tentative and incomplete as activities to ensure visibility and increase engagement may evolve over time depending on specific partner roles.

[28] https://www.caeconference.com/exibitors.html with link to http://www.max-centre.eu/ .

3rd-Party events: HPC Ecosystem September 2020 to November 2021		
Event	**Date (Q+YR)**	**Stakeholder Type and Visibility**
NVIDIA GTC 2020: Deep Learning and AI Conference[29]	Q4-2020, virtual	HW manufacturers, HPC actors, industry.
Supercomputing 2020 (SC20)[30]	Q4-2020, virtual	HPC; industry; academia.
CAE Conference and Exhibition	Q4-2020, virtual	Industry. Visibility on the CAE website (exhibitors) and during the event. Social media campaign benefiting from the joint presence of FocusCoE and Excellerat.
European Researchers' Night 2020[31]	Q4-2020, virtual	General public. Visibility through the livestreaming of CNR video. Social media highlights. Event announcement on MAX website.
HiPEAC Conference 2021[32]	Q1-2021, virtual	HPC community: Industry; Academia and Research. Highlights through social media with announcement on MAX website.
European Materials Modelling Conference (EMMC)	Q1-2021, virtual	Industry (Materials Science). Highlights through social media with announcement on MAX website.
EuroHPC Summit Week	Q1-2021	HPC community: Academia and Research; Industry. Especially synergies established with EU institutions and ecosystems. Visibility at the event. Website announcement and social media highlights throughout the event.
EUSEW 2021	Q2-2021	Policy makers, Academia and Research; industry, General Public (Energy Days) Visibility at the event. Website announcement and social media highlights throughout the event.

[29] https://www.nvidia.com/en-us/gtc/.
[30] https://sc20.supercomputing.org/.
[31] https://ec.europa.eu/research/mariecurieactions/news/results-msca-night-2020_en.
[32] https://www.hipeac.net/2021/spring-virtual/#/.

International Supercomputing Conference (ISC)[33]	Q2-2021	HPC community, including academia and research; industry. Visibility at the event. Website announcement and social media highlights throughout the event.
PASC21 Conference 2021[34], co-sponsored by ACM and CSCS	Q3-2021	HPC community: Academia and Research. Visibility at the event. Website announcement and social media highlights throughout the event.
Psi-K Conference 2021	Q3-2021	Academia and Research. Visibility through partner organization. Visibility at the event. Website announcement
Graphene Week 2021	Q3-2021	Academia and Research. Visibility at the event. Website announcement and social media highlights throughout the event.

Table 5: Sample of targeted 3rd-party Events.

4.5 Editorial Plan

The Plan plots a core set of activities taking place in M25-36. Given the on-going COVID-19 pandemic, the plan is considered a living document that will be regularly updated in concert with the MAX consortium over the remainder of the project, detailing specific roles and responsibilities.

Timeline	Activity Planned	Partners Involved
November 2020	BigDFT Webinar (flagship code series). Publication of highlights and insights on the website. SMART social media campaign.	CNR, Trust-IT Webinar partners
November 2020	European Researchers' Night 2020 MAX participation includes the live streaming of a dedicated video exploring the use of supercomputing for scientific	CNR

[33] https://www.ics-conference.org/.
[34] https://pasc21.pasc-conference.org/.

	research.	
Late November-early December 2020	CAE vExhibition with FocusCoE and Excellerat: Promotion of booth materials through social media SMART campaign.	Trust-IT, CNR, ICN2, E4, CINECA
December 2020-January 2021	Graphically-designed Webinar Impact Report: Collective impacts of the flagship code webinar series. Promotional campaign, also targeting synergies with EU institutions and environment.	CNR, SISSA, CINECA, EPFL, ETH, ICN2, JUELICH, CEA, Trust-IT
December 2020	SMART promotional campaign on recent MAX publications with dedicated banners and news pieces.	CNR, Trust-IT
January 2021	HiPEAC Conference 2021. Promotional campaign on highlights and MAX presence.	tbc
January 2021	1st MAX podcast with extracted soundbites and Twitter banners on takeaways.	tbc
January 2021	Collection and production of Testimonial Cards. SMART promotional Campaign.	Trust-IT, CNR and partners with user testimonials.
February 2021	SMART promotional campaign on MAX assets, Part 1 - Flagship codes with dedicated banners	Trust-IT, CNR
February 2021	User stories part 1 (based on a new template: who they are, what they do, how they use MAX, how they benefit). SMART promotional Campaign.	Selected partners, CNR, Trust-IT
February 2021	MAX Webinar SMART promotional and recruitment campaign	Selected panellists, CNR, Trust-IT
March 2021	European Materials Modelling Conference	tbc

	(EMMC)	
March 2021	EuroHPC Summit Week (EHPCSW) 2021	tbc
March 2021	MAX Press Release	CNR, Trust-IT
April 2021	User stories part 2 SMART promotional Campaign.	tbc
May 2021	MAX Webinar SMART promotional and recruitment campaign	tbc
May 2021	MAX Podcast	tbc
May 2021	SMART promotional campaign on MAX assets, Part 2	tbc
June 2021	International Supercomputing Conference (ISC) 2021	tbc
June 2021	MAX Webinar SMART promotional and recruitment campaign	tbc
July 2021	User stories part 3 SMART promotional Campaign.	tbc
July 2021	PASC21 Conference 2021	tbc
August 2021	Psi-K Conference 2021	EPFL, MAX as a whole
September 2021	Graphene Week	tbc
September 2021	MAX Webinar SMART promotional and recruitment campaign	Selected panellists, CNR, Trust-IT
September 2021	SMART promotional campaign on MAX assets, Part 2	tbc
October 2021	MAX Podcast	tbc

October 2021	MAX Collection of User Stories as a graphically designed booklet	CNR, Trust-IT
October 2021	Graphically designed booklet on MAX Assets	CNR, Trust-IT, all partners
November 2021	Final MAX Press Release	CNR, Trust-IT
November 2021	MAX Final Showcase Event (tbc) Recruitment campaign. Showcase package, e.g. interviews; banners and fliers.	tbc
November 2021	MAX Final Workshop Website showcase articles. SMART social media campaign. Highlights from final year (Achievement Booklet). Interviews, including end-user stories and special series of science@MAX website features, e.g. on the transition towards exascale, flagship codes, citations, publications.	CNR, Trust-IT, partners from WP1-10.
November 2021	MAX Results Package submitted to CORDIS	CNR, Trust-IT

Table 6: Summary of Planned Activities at the time of writing this report.

5. Monitoring Impacts

When talking about impact, we must highlight that 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.

In D9.2 "Impact Assessment Report, mid-term version" (M18) we showed the assessment of MAX impact according to objectives above. For example, 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. Codes received in scientific publications about 6200+ citations in the period 01/2019 - 09/2020 (over 10000 estimated single downloads/year). In the same period about 1000+ participants attended MAX training activities.

We showed how effective and lively relationships in Europe between main initiatives and MAX exist, including 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. We highlighted the role of MAX in many domain specific initiatives such as e.g. the Psi-k, Cecam and the Graphene flagship project. Along with this, the impact and networking with academia, industry and other stakeholders has been discussed, and will be again in final D9.4 "Impact Assessment Report, final version" (M36).

5.1 Monitoring of Impacts of Communication activities

Beside this overall and full assessment, impacts achieved through the implementation of the M25-36 communication plan will be monitored in diverse ways: infographics on the overall performance (see Fig. 21); infographics on core activities (e.g. webinars, see Fig. 22); dashboard analytics comprising regularly updated datasets. The figures below are examples of the impacts that will be monitored during M25-36 based on achievements to date.

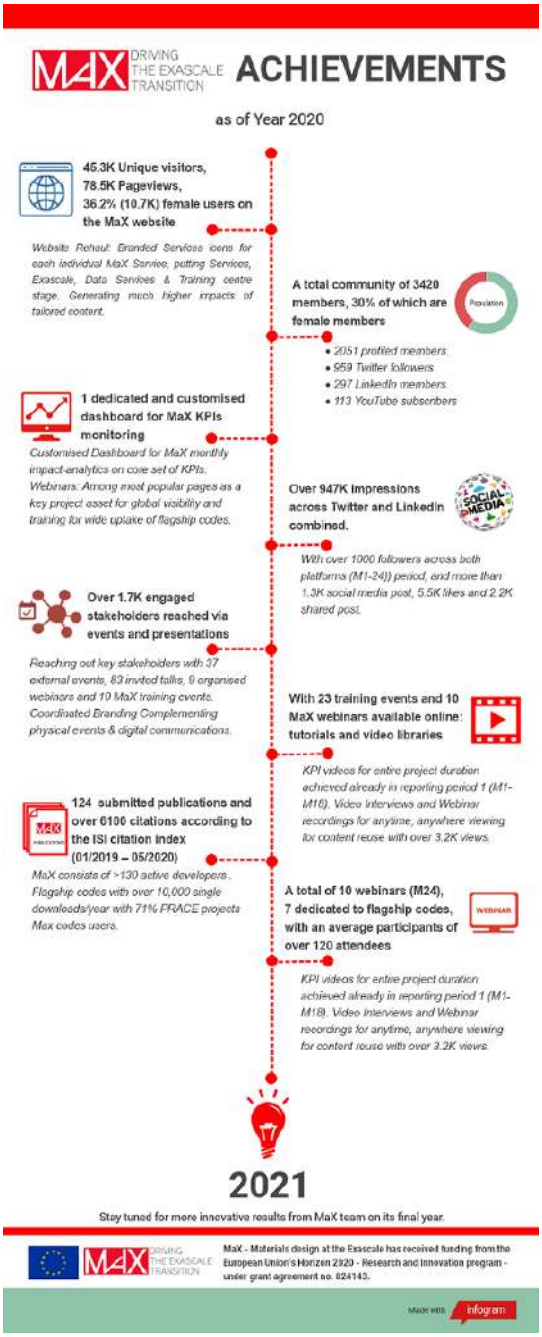


Figure 21: MAX Achievements Infographics: presentation of the main impacts for the period M1-24. Such an activity will be included in the plan for M25-36, highlighting the major achievements of MAX.

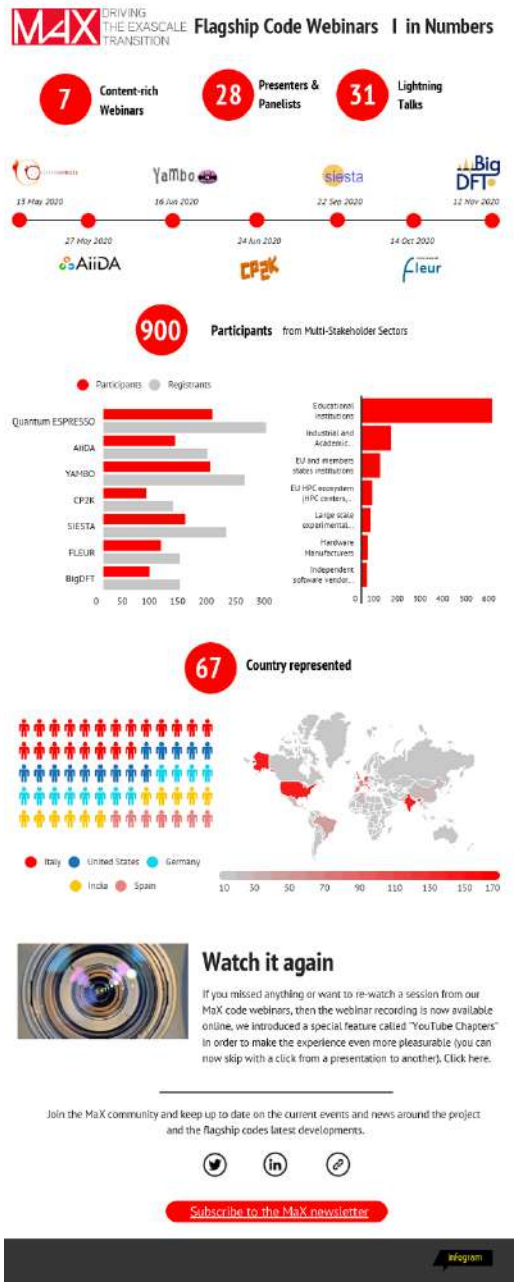


Figure 22: MAX Webinar Achievements Infographics: presentation of overall impacts of the flagship code webinar series.

5.1.1 Dashboard Monitoring of Impacts

These next figures show the impacts of the targets monitored through the customized Dashboard, which tracks website and social media performance. The statistics refer to the period January 2019 to November 2020.

Dashboard - Website Impacts: The number of pageviews and the most popular pages. Details on number of users, sessions; average session duration; page views and average time on page, as well as data on new and returning visitors and gender balance. Pageviews and sessions can also be assessed for a given period of time to gauge impacts of campaigns and new web content. The Dashboard analysis also includes data on traffic (e.g. direct or referral traffic) and country ranking.

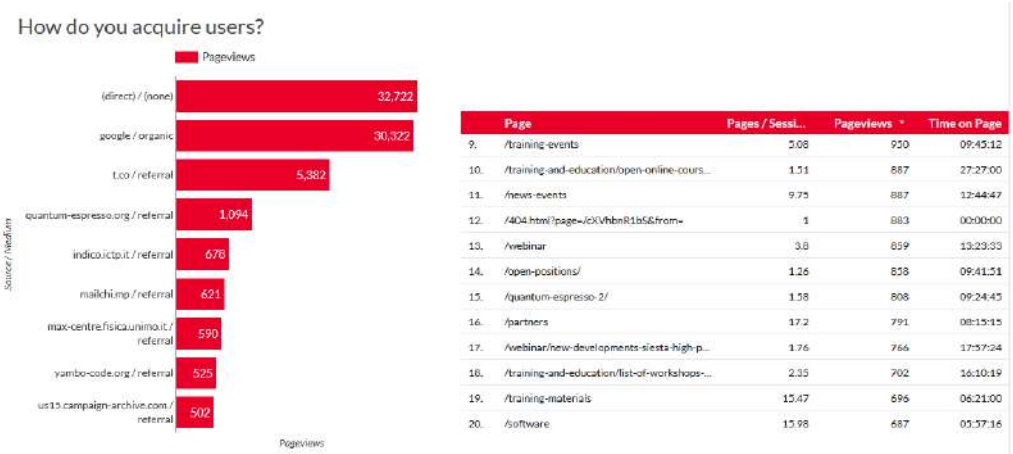


Figure 23: Dashboard: Website Statistics - Pageviews.

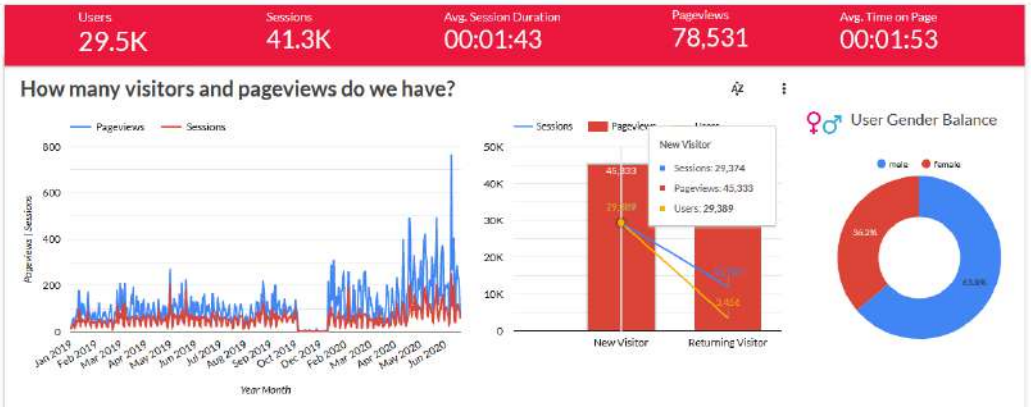


Figure 24: Dashboard: Website Statistics - Usage Data.

Dashboard - Social Media: **Twitter**. Statistics include the number of followers, Tweets, likes, retweets, latest sample of Tweets, country coverage with ranking, sectors.

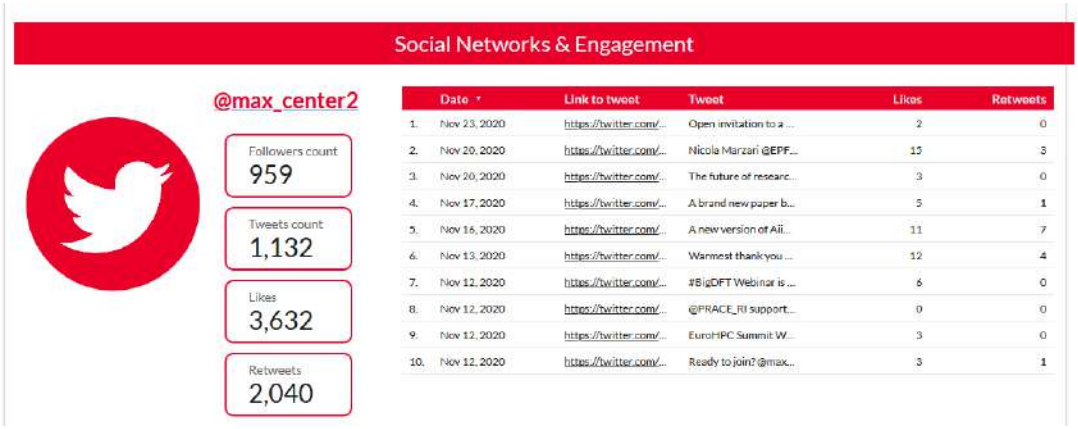


Figure 25: Dashboard: Twitter engagement.

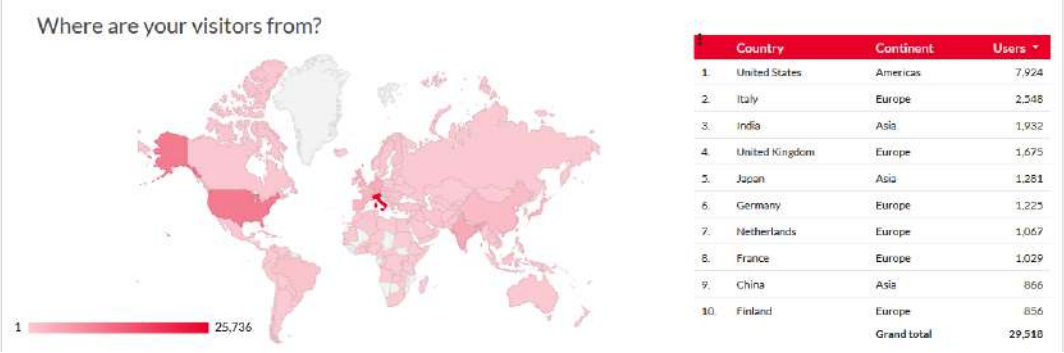


Figure 26: Dashboard: Twitter Country coverage ranking.

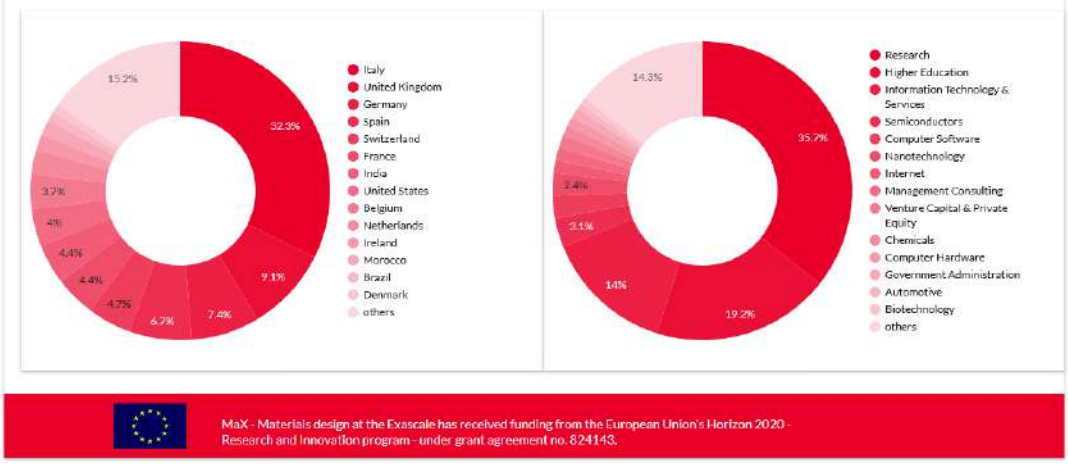
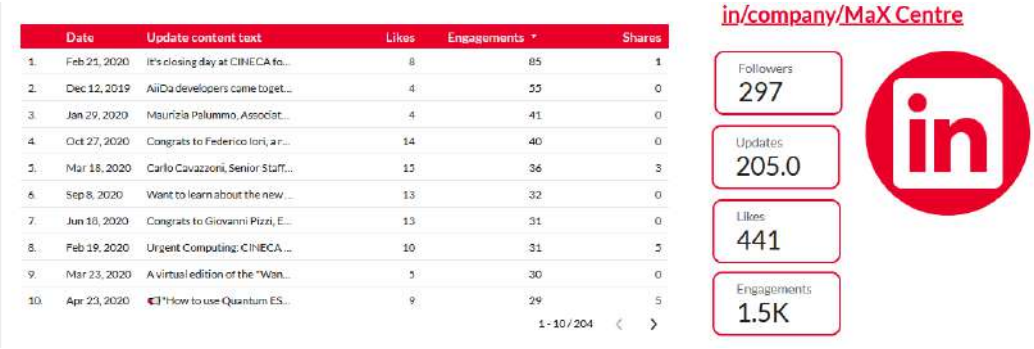


Figure 27: Dashboard: Twitter Country and Sector Breakdown.

Dashboard - Social Media: **LinkedIn**. Statistics include followers, updates, likes, engagements, country coverage and industry breakdown.



	Date	Update content text	Likes	Engagements	Shares
1.	Feb 21, 2020	It's closing day at CINECA fo...	8	85	1
2.	Dec 12, 2019	AiiDa developers come toget...	4	55	0
3.	Jan 29, 2020	Maurizia Palummo, Associat...	4	41	0
4.	Oct 27, 2020	Congrats to Federico Iori, a r...	14	40	0
5.	Mar 18, 2020	Carlo Cavazzoni, Senior Staff...	15	36	3
6.	Sep 8, 2020	Want to learn about the new ...	13	32	0
7.	Jun 18, 2020	Congrats to Giovanni Pizzi, E...	13	31	0
8.	Feb 19, 2020	Urgent Computing: CINECA ...	10	31	5
9.	Mar 23, 2020	A virtual edition of the "Wan...	5	30	0
10.	Apr 23, 2020	"How to use Quantum ES...	9	29	5

1 - 10 / 204

Figure 28: Dashboard: LinkedIn Engagement.

6. Conclusions and Next Steps

This "Communication & Dissemination Strategy & Stakeholder Engagement Plan, Final version" (M30) strongly relies on the former D9.1 "Communication & dissemination Strategy & Stakeholder Engagement Plan" and updates and strengthens it. A huge effort has been done by MAX in communication and dissemination activities, both at a consortium and at an individual level. The several aspects of MAX activity, from code development to co-design, from uptaking of the different groups of stakeholders to training for different-level of expertise, from participating to the European HPC ecosystem to being active in the materials modelling domain, need to be reflected in our communication activities as a return on public investment and as a core asset of our Centre of Excellence and its strive towards excellence. The WP9 leader partner Trust-IT has so far led activities and has worked in close connection with the WP8 and WP10 and their leader partner Cnr and has received continuous and steady support from the MAX Management Team. All partners and WPs have contributed to the development of MAX communication actions and have led several dissemination activities on their own, giving the consortium a well-known and recognized position in the relevant environments.

In the second part of the action, communication and dissemination will focus on the results we achieve and the contribution we give to the ecosystem. We will endeavour to make our achievements useful for the different stakeholder communities and for the uptake from industry and academia. In brief, our plan foresees to:

- Adopt an inclusive approach working towards the final phase of MAX.
- Tighten the collaboration with the other Work Packages in order to achieve a more harmonised, timely and exhaustive degree of Communication and Dissemination.
- Reengineering of the whole Communication Strategy and Events Management as a prompt response to the side-effects of the Covid-19 pandemic.

The consolidation of the existing communication strategy and the development of new actions to make us recognized, reliable and prominent in the relevant areas will permit us to fully accomplish our communication and impact goals.

ANNEX 1 - List of Acronyms

Acronym	Description
AiiDA	Automated Interactive Infrastructure and Database for computational science
BSC	Barcelona Supercomputing Centre / Centro Nacional de Supercomputación
CEA	Commissariat à l'Énergie Atomique et aux Énergies
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
CSCS	Swiss National Supercomputing Centre
D8.2	First report on Training and Education
D9.1	MAX Communication & dissemination Strategy & Stakeholder Engagement Plan
D9.2	Impact Assessment Report, mid-term version
EOSC	European Open Science Cloud
EPFL	Ecole Polytechnique Fédérale de Lausanne
ETHZ	Eidgenössische Technische Hochschule Zürich
EMMC	The European Materials Modelling Council
EU	European Union
FLEUR	Full-potential Linearised augmented plane wave in EURope
GPU	Graphics Processing Unit

HPC	High Performance Computing
HTC	High Throughput Computing
HPDA	High Performance Data analysis
HW	Hardware
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	Materials design at the eXascale
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
SISSA	Scuola Internazionale Superiore di Studi Avanzati, Trieste
SMART	Specific, Measurable, Achievable, Realistic and Timed
SME	Small Medium Enterprise
WP	Work Package

ANNEX 2 - List of Scientific Publications

CATEGORY 1: Scientific Publications targeting the HPC community [HPC centres]
(as defined in D9.1 point 2.4)

1. *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

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

3. *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

4. *AiiDA 1.0, a scalable computational infrastructure for automated reproducible workflows and data provenance*, S. P. Huber, S. Zoupanos, M. Uhrin, L. Talirz, L. Kahle, R. Häuselmann, D. Gresch, T. Müller, A. V. Yakutovich, C. W. Andersen, F. F. Ramirez, C. S. Adorf, F. Gargiulo, S. Kumbhar, E. Passaro, C. Johnston, A. Merkys, A. Cepellotti, N. Mounet, N. Marzari, B. Kozinsky, and G. Pizzi, Sci Data 7, 300 (2020) DOI: https://doi.org/10.1038/s41597-020-00638-4

5. *ELSI -- An Open Infrastructure for Electronic Structure Solvers*, V. Wen-zhe Yu, C. Campos, W. Dawson, A. García, V. Havu, B. Hourahine, W. P Huhn, M. Jacquelin, W. Jia, M. Keçeli, R. Laasner, Y. Li, Lin Lin, J. Lu, J. Moussa, J. E Roman, Á. Vázquez-Mayagoitia, C. Yang, V. Blum, Comp. Phys. Comm. Volume 256, 107459 (2020) DOI: https://doi.org/10.1016/j.cpc.2020.107459

6. *Workflows in AiiDA: Engineering a high-throughput, event-based engine for robust and modular computational workflows*, M. Uhrin, S. P. Huber, J. Yu, N. Marzari, and G.Pizzi, Computational Materials Science 187, 110086 (2020) DOI: https://doi.org/10.1016/j.commatsci.2020.110086

7. *Countdown Slack: A Run-Time Library to Reduce Energy Footprint in Large-Scale MPI Applications*, D. Cesarini, A. Bartolini, A. Borghesi, C. Cavazzoni, M. Luisier and L. Benini, IEEE Transactions on Parallel and Distributed Systems, vol. 31, no. 11, pp. 2696-2709 (2020) DOI: https://doi.org/10.1109/TPDS.2020.3000418

8. *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

9. *The CECAM Electronic Structure Library and the modular software development paradigm*, M. J. T. Oliveira, N. Papior, Y. Pouillon, V. Blum, E. Artacho, D. Caliste, F. Corsetti, S. de Gironcoli, A. M. Elena, A. Garcia, V. M. Garcia-Suarez, L. Genovese, W. P. Huhn, G. Huhs, S. Kokott, E. Kucukbenli, A. H. Larsen, A. Lazzaro, I. V. Lebedeva, Y. Li, D. Lopez-Duran, P. Lopez-Tarifa, M. Luders, M. A. L. Marques, J. Minar, S. Mohr, A. A. Mostofi, A. O'Cais, M. C. Payne, T. Ruh, D. G. A. Smith, J. M.

Soler, D. A. Strubbe, N. Tancogne-Dejean, D. Tildesley, M. Torrent, and V. Wen-zhe Yu, J. Chem. Phys. 153, 024117 (2020) DOI: https://doi.org/10.1063/5.0012901

10. *Workflows in AiiDA: Engineering a high-throughput, event-based engine for robust and modular computational workflows*, M. Uhrin, S. P. Huber, J. Yu, N. Marzari, and G.Pizzi, Computational Materials Science 187, 110086 (2020) DOI: https://doi.org/10.1016/j.commatsci.2020.110086

CATEGORY 2: Scientific Publications targeting end-users of materials simulations and code developers [codes & ecosystem developers]
(as defined in D9.1 point 2.4)

11. *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

12. *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

13. *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

14. *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

15. *Spin States Protected from Intrinsic Electron–Phonon Coupling Reaching 100 ns Lifetime at Room Temperature in MoSe2*, M. Ersfeld, F. Volmer, P. M. M. C. de Melo, R. de Winter, M. Heithoff, Z. Zanolli, C. Stampfer, M. J. Verstraete, and B. Beschoten, Nano Lett. 19, 6, 4083-4090 (2019) DOI: https://doi.org/10.1021/acs.nanolett.9b01485

16. *Valley-engineering mobilities in 2D materials*, T. Sohier, M. Gibertini, D. Campi, G. Pizzi, and N. Marzari, Nano Lett. 19, 3723−3729 (2019) DOI: https://doi.org/10.1021/acs.nanolett.9b00865

17. *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

18. *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

19. *Equipartition of Energy Defines the Size− Thickness Relationship in Liquid-Exfoliated Nanosheets*, C. Backes, D. Campi, B. M. Szydłowska, K. Synnatschke, E. Ojala, F. Rashvand, A. Harvey, A. Griffin, Z. Sofer, N. Marzari, J. N. Coleman, and D. D. O'Regan, ACS Nano 13, 7050−7061 (2019) DOI: 10.1021/acsnano.9b02234

20. *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

21. *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

22. *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

23. *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

24. *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

25. *Pump-driven normal-to-excitonic insulator transition: Josephson oscillations and signatures of BEC-BCS crossover in time-resolved ARPES*, E. Perfetto, D. Sangalli, A. Marini, and G. Stefanucci, Phys. Rev. Materials 3, 124601 (2019) DOI: https://doi.org/10.1103/PhysRevMaterials.3.124601

26. *Optical Properties of Lead-Free Double Perovskites by Ab Initio Excited-State Methods*, M. Palummo, E. Berrios, D. Varsano, and G. Giorgi, ACS Energy Lett. 2020, 5, 2, 457–463 (2020) DOI: https://doi.org/10.1021/acsenergylett.9b02593

27. *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

28. I*nvestigation 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

29. *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

30. *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

31. *Emergent dual topology in the three-dimensional Kane-Mele Pt2HgSe3*, A. Marrazzo, N. Marzari, and M. Gibertini, Physical Review Research 2, 012063 (2020) DOI: https://doi.org/10.1103/PhysRevResearch.2.012063

32. *Intrinsic edge excitons in two-dimensional MoS2*, P. D'Amico, M. Gibertini, D. Prezzi, D. Varsano, A. Ferretti, N. Marzari, and E. Molinari, Physical Review B 101, 161410 (2020) DOI: https://doi.org/10.1103/PhysRevB.101.161410

33. *Fermi surface electron–hole instability of the (TMTSF)2PF6 Bechgaard salt revealed by the first-principles Lindhard response function*, B. Guster, A. Pruneda, P. Ordejón, E. Canadell, J. P. Pouget, Journal of Physics: Condensed Matter 32, 34 (2020), DOI: https://dx.doi.org/10.1088/1361-648X/ab8522

34. *CP2K: An electronic structure and molecular dynamics software package - Quickstep: Efficient and accurate electronic structure calculations*, T.D. Kühne, M. Iannuzzi, M. Del Ben, V.V. Rybkin, P. Seewald, F. Stein, T. Laino, R. Z. Khaliullin, O. Schütt, F. Schiffmann, D. Golze, J. Wilhelm, S. Chulkov, M. Hossein Bani-Hashemian, V. Weber, U. Borštnik, M. Taillefumier, A.S. Jakobovits, A. Lazzaro, H. Pabst, T. Müller, R. Schade, M. Guidon, S. Andermatt, N. Holmberg, G. K. Schenter, A. Hehn, A. Bussy, F. Belleflamme, G. Tabacchi, A. Glöß, M. Lass, I. Bethune, C.J. Mundy, C. Plessl, M. Watkins, J. VandeVondele, M. Krack, and J. Hutter, J. Chem. Phys. 152, 194103 (2020) DOI: https://doi.org/10.1063/5.0007045

35. *Magneto-optical response of chromium trihalide monolayers: chemical trends*, A. Molina-Sánchez, G. Catarina, D. Sangalli, and J. Fernández-Rossier, J. Mater. Chem. C, 2020,8, 8856-8863 (2020) DOI: https://doi.org/10.1039/D0TC01322F

36. *Automated high-throughput Wannierisation*, V. Vitale, G. Pizzi, A. Marrazzo, J. Yates, N. Marzari, and A. Mostofi, npj Computational Materials 6, 66 (2020) DOI: https://doi.org/10.1038/s41524-020-0312-y

37. *Halide Pb-free Double–Perovskites: Ternary vs. Quaternary Stoichiometry*, M. Palummo, D. Varsano, E. Berríos, K. Yamashita and G. Giorgi, Energies 13, 3516 (2020) DOI: https://doi.org/10.3390/en13143516

38. *Heat and charge transport in H2O at ice-giant conditions from ab initio MD simulations*, F. Grasselli, L. Stixrude, and S. Baroni, Nat Commun 11, 3605 (2020) DOI: https://doi.org/10.1038/s41467-020-17275-5

39. *Unit cell restricted Bloch functions basis for first-principle transport models: Theory and application*, M. G. Pala, P. Giannozzi, and D. Esseni, Phys. Rev. B 102, 045410 (2020) DOI: https://doi.org/10.1103/PhysRevB.102.045410

40. *Observation of an Excitonic Mott Transition through Ultrafast Core-cum-Conduction Photoemission Spectroscopy*, M. Dendzik, R. P. Xian, E. Perfetto, D. Sangalli, D. Kutnyakhov, S. Dong, S. Beaulieu,

T. Pincelli, F. Pressacco, D. Curcio, S. Y. Agustsson, M. Heber, J. Hauer, W. Wurth, G. Brenner, Y. Acremann, P. Hofmann, M. Wolf, A. Marini, G. Stefanucci, L. Rettig, and R. Ernstorfer, Phys. Rev. Lett. 125, 096401 (2020) DOI: https://doi.org/10.1103/PhysRevLett.125.096401

41. *Self-consistent screening enhances stability of the nonequilibrium excitonic insulator phase*, E. Perfetto, A. Marini, G. Stefanucci, Phys. Rev. B 102, 085203 (2020) DOI: https://doi.org/10.1103/PhysRevB.102.085203

42. *Exciton-Phonon Interaction and Relaxation Times from First Principles*, H. Chen, D. Sangalli, M. Bernardi, Phys. Rev. Lett. 125, 107401 (2020) DOI: https://doi.org/10.1103/PhysRevLett.125.107401

43. *Vibrational signature of the graphene nanoribbon edge structure from high-resolution electron energy-loss spectroscopy*, N. Cavani, M. De Corato, A. Ruini, D. Prezzi, E. Molinari, A. Lodi Rizzini, A. Rosi, R. Biagi, V. Corradini, X.-Y. Wang, X. Feng, A. Narita, K. Muellen, and V. De Renzi, Nanoscale 12, 19681-19688 (2020) DOI: https://doi.org/10.1039/D0NR05763K

44. *Surface chemistry effects on work function, ionization potential and electronic affinity of Si(100), Ge(100) surfaces and SiGe heterostructures*, I. Marri, M. Amato, M. Bertocchi, A. Ferretti, D. Varsano and S. Ossicini, Phys. Chem. Chem. Phys. 22, 25593-25605 (2020) DOI: https://doi.org/10.1039/D0CP04013D

45. *Real-time modelling of Optical orientation in GaAs: generation and decay of the degree of spin polarization*, M. D'Alessandro and D. Sangalli, Phys. Rev. B 102, 104437 (2020) DOI: https://doi.org/10.1103/PhysRevB.102.104437

46. *Electrosorption at metal surfaces from first principles*, N. G. Hörmann, N. Marzari, and K. Reuter, npj Computational Materials 6, 136 (2020) DOI: https://doi.org/10.1038/s41524-020-00394-4

47. *Electron energy loss spectroscopy of bulk gold with ultrasoft pseudopotentials and the Liouville-Lanczos method*, O. Motornyi, N. Vast, I. Timrov, O. Baseggio, S. Baroni, and A. Dal Corso, Physical Review B 102, 035156 (2020) DOI: https://doi.org/10.1103/PhysRevB.102.035156

48. *Material systems for FM-/AFM-coupled skyrmions in Co/Pt-based multilayers*, H. Jia, B. Zimmermann, M. Hoffmann, M. Sallermann, G. Bihlmayer, and S. Blügel, Phys. Rev. Materials 4, 094407 (2020) DOI: https://doi.org/10.1103/PhysRevMaterials.4.094407

49. *Ab initio studies of the optoelectronic structure of undoped and doped silicon nanocrystals and nanowires: the role of size, passivation, symmetry and phase*, S. Ossicini, I.Marri, M. Amato, M. Palummo, E. Canadell, and R. Rurali, Faraday Discuss. 222, 217 (2020) EOI: https://doi.org/10.1039/C9FD00085B

Preprint papers

- *Thermal Evolution of Uranus with a Frozen Interior*, L. Stixrude, S. Baroni, F. Grasselli
- *Oxidation states, Thouless' pumps, and anomalous transport in non-stoichiometric ionic conductors*, P. Pegolo, F. Grasselli, and S. Baroni

- *AiiDAlab -- an ecosystem for developing, executing, and sharing scientific workflows*, A. V. Yakutovich, K. Eimre, O. Schütt, L. Talirz, C. S. Adorf, C. W. Andersen, E. Ditler, D. Du, D. Passerone, B. Smit, N. Marzari, G. Pizzi, and C. A. Pignedoli

ANNEX 3 - List of Events

CATEGORY 1: Scientific conferences and workshops on HPC, targeting mostly the HPC community and HW stakeholders [HPC centres, technology partners]
(as defined in D9.1 point 2.4)

Event Name	Date (dd/mm/yyyy)	Where (City, Country)	Participant Name	Node	Speaker	title of the talk/poster
PRACE PCP DAVIDE OpenPower cluster: user experiences and scientific cases	10/12/2018	Casalecchio di Reno (IT)	Carlo Cavazzoni Fabio Affinito Fabrizio Magugliani	CINECA E4	Carlo Cavazzoni Fabio Affinito Fabrizio Magugliani	The PRACE PCP in the european framework - DAVIDE: a success story - Fabrizio Magugliani
HiPEAC 2020	20-22/01/2019	Bologna (IT)	Fabrizio Magugliani Conrad Hillairet	E4 Arm	Fabrizio Magugliani	Stated the importance of developing materials (as intended in MaX) for the competitiveness of the European industrial ecosystem
PRACE 15th Advanced School on Parallel Computing	11-15/02/2019	Casalecchio (IT)	Carlo Cavazzoni	CINECA		
European HPC Summit Week 2019	13-17/05/2019	Poznan (PL)	Carlo Cavazzoni Sebastiaan Huber Fabrizio Magugliani Elisa Molinari Luisa Neri	CINECA EPFL E4 CNR Nano	Carlo Cavazzoni Sebastiaan Huber	CC: Grand challenge applications: technical requirements for the exascale era; SH: 1st European Communities Workshop on Exascale Computing Focus on High Performance Data Analytics
HPC for Industry 4.0	21-23/05/2019	Milano (IT)	Elisa Molinari Fabrizio Magugliani	CNR Nano E4		EM: MaX: screening and designing materials with HPC; FM: Why HPC is key for the competitiveness of the industry (and particularly for SMEs)
PASC19	12-14/06/2019	Zurich (CH)	Zeila Zanolli Carlo Cavazzoni Andrea Ferretti	CINECA ICN2 CNR Nano	Carlo Cavazzoni Andrea Ferretti	CC: Prediction of Time-to-Solution in Material Science Simulations Using Deep Learning; AF Poster: Many-Body Perturbation Theory Towards the #Exascale: Yambo on #GPUs"
ISC19	16-20/06/2019	Frankfurt (DE)	Fabrizio Magugliani	E4		

Campus Party Italia 3	26/07/2019	Milano (IT)	Carlo Cavazzoni	CINECA	Carlo Cavazzoni	The energy efficiency challenge for the future of computing
ApplePies Applications in Electronics Pervading Industry, Environment and Society	11-13/09/2019	Pisa (IT)	Fabrizio Magugliani Federico Ficarelli	E4 CINECA	Fabrizio Magugliani Federico Ficarelli	Round Table: Trend in Italy on EuroHPC & the European Processor Initiative
SC19	17-22/11/2019	Denver, CO (USA)	Filippo Spiga Carlo Cavazzoni Fabrizio Magugliani	Arm CINECA E4		
HiPEAC 2020	20-22/01/2019	Bologna (Italy)	Fabrizio Magugliani Conrad Hillairet	E4 Arm		
EuroHPC Summit Week - **EVENT CANCELLED, but everything was defined, also the MaX Session (to be held on 2021)**	23-27/03/2020	online	Elisa Molinari Andrea Ferretti Claudia Cardoso Carlo Cavazzoni Joost VandeVondele	CNR Nano CINECA ETHZ	Elisa Molinari Andrea Ferretti Claudia Cardoso Carlo Cavazzoni Joost VandeVondele	Computational Materials Science towards the exascale: performance portability and use cases
High Performance Innovation Conference	30/03/2020	online	Stephan Mohr	BSC	Stephan Mohr	Millions to hundreds of millions of simulations are needed to optimise the properties and performances of a material or a device
HPC-CH 2020 Forum on Access Abstraction to HPC Resources	22/10/2020	online	Giovanni Pizzi	EPFL	Giovanni Pizzi	Reproducible high-throughput HPC workloads with AiiDA

CATEGORY 2: Scientific conferences and workshops in materials science and engineering, physics and chemistry, targeting mostly end-users of materials simulations in industry and academia [codes & ecosystem developers]
(as defined in D9.1 point 2.4)

Event Name	Date (dd/mm/yyyy)	Where (City, Country)	Participant Name	Node	Speaker	title of the talk/poster
BDEC Conference	10/12/2018		Thierry Deutsch	CEA		
Material Science codes on innovative HPC architectures: from electronic structure to spectra with Quantum ESPRESSO and Yambo	03-05/12/2018	Casalecchio di Reno (IT)		CINECA CNR Nano and ISM	Fabio Affinito Pietro Bonfà Andrea Ferretti Andrea Marini	
Third AiiDA Coding Week	03-07/12/2018	Fiesch (CH)	Giovanni Pizzi Spyros Zoupanos & code developers	EPFL		
Invited talk @ Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie	16/01/2020	Paris (FR) @ Sorbonne	Stefano Baroni	SISSA		Heat transport in water at icy-giants conditions from ab initio MD simulations
19th International Workshop on Computational Physics and Material Science: Total Energy and Force Methods	09-11/01/2019	Trieste (IT) @ ICTP	Stefano Baroni Stefano De Gironcoli Paolo Giannozzi Andrea Ferretti Daniele Varsano Claudia Cardoso Nicola Marzari	SISSA CNR Nano EPFL	Nicola Marzari	Computational materials discovery: good data vs big data
QE developers meeting 2019	07-08/01/2019	Trieste (IT) @ SISSA	Paolo Giannozzi Pietro Bonfà	SISSA CINECA CNR IOM		
Yambo and QE developers meeting	14/01/2019	Casalecchio (IT) @ CINECA	Code developers			
Towards Reality in Nanoscale Materials X	12/02/2019	Levi (FI)	Zeila Zanolli (Invited Talk)	ICN2	Zeila Zanolli	Spintronics at the interface
Open Science Days 2019	02/02/2019	Berlin (DE)	Giovanni Pizzi	EPFL	Giovanni Pizzi	Open Science Platform for Materials Science: AiiDA and the Materials Cloud
Nano Colloquia 2019	27/03/2019	Modena (IT)	Andrea Ferretti	CNR Nano	Andrea Ferretti	From koopmans-compliant functionals to a functional theory of the spectral density

DPG Spring Meeting of the Condensed Matter Section	31/03- 05/04/2019	Regensburg (DE)	Vasily Tseplyaev Uliana Alekseeva Giovanni Pizzi	Juelich EPFL	Vasily Tseplyaev Uliana Alekseeva Giovanni Pizzi	VT: Investigation of Fe/Pt (110) magnetic structure by first-principles methods; UA: Parallelization and Acceleration of the FLEUR Code: New Possibilities for All-electron Density Functional Theory; GP: Presentation1: Robust automatic Wannierisation; Presentation2: Reproducible massive calculations and data sharing with AiiDA and the Materials Cloud
International Winterschool on Electronic Properties of Novel Materials	13-15/03/2019	Kirchberg in tirol (Austria)	Deborah Prezzi	CNR		
SISSA seminar	17/04/2019	Trieste (IT) @ SISSA	Andrea Ferretti	CNR	Andrea Ferretti	Koopmans compliance: Towards a functional theory of the spectral density
Lavoisier Discussion on Quantum Simulation	8-9/05/2019	Barcelona (ES)	Zeila Zanolli Nicola Marzari Daniele Varsano	ICN2 EPFL CNR Nano	Zeila Zanolli Nicola Marzari Daniele Varsano	ZZ: Ab initio exciton & phonon dynamics in Transition Metal Dichalcogenides; NM: Modelling thermal transport in 2D materials; DV: Exciton instabilities in monolayer T'-MoS2 and bulk MoS2 under pressure
Green's function methods: the next generation 4	14-17/05/2019	Lausanne (CH)	Davide Sangalli	CNR ISM	Davide Sangalli	An ab-initio approach to describe coherent and non-coherent exciton dynamics in pump and probe (P&p) experiments
ICTP Caribbean School on Materials for Clean Energy	30/05-05/06/2019	Cartagena de Indias, Colombia	Stefano Baroni	SISSA		Thermal transport from first principles
Nano Materials & Devices 2019	04-08/06/2019	Paestum (IT)	Zeila Zanolli	ICN2	Zeila Zanolli	Spintronics at the interface
NanoInnovation 2019	11-14/06/2019	Rome (IT)	Mariella Ippolito	CINECA		
Optimade conference	11/06/2019	Lausanne (CH)	Giovanni Pizzi	EPFL	Giovanni Pizzi	Optimade implementation in AiiDA

ORQUID workshop	17-19/06/2019	Castelldefels (ES)	Deborah Prezzi	CNR		
Conference on Nanophononics: Bridging Statistical Physics, Molecular Modeling, and Experiments	24-28/06/2019	Trieste (IT) @ ICTP	Stefano Baroni	SISSA		Ab initio simulation of heat transport in liquids and glasses
International Conference on Multi-Scale Modelling and Simulation of Materials - ICM3	1-5/07/2019	Ningbo, China	Stefano Baroni	SISSA		Ab initio simulation of heat transport in liquids and glasses
Common Format for Materials Science Data	08/07/2019	Berlin (DE)	Giovanni Pizzi	EPFL	Giovanni Pizzi	Data and metadata in AiiDA and the Materials Cloud
ICIAM 2019	15-19/07/2019	Valencia (ES)	Stefano De Gironcoli Alberto Garcia	SISSA ICN2	Alberto Garcia	AG: New features and performance improvements in the SIESTA code
SiSPAD - International conference on Simulation of semiconductor processes and devices	3/9/2019	Udine (IT)	Paolo Giannozzi	CNR IOM	Paolo Giannozzi	Basics of density-functional theory simulations: opportunities and limits
MSSC2019@London - Ab initio Modelling in Solid State Chemistry	16-20/09/2019	London (UK)	Andrea Ferretti	CNR		
XVIII meeting of the Brazilian Materials Research Society	22-26/09/2019	Balneário Camboriú, Brazil	Stefano Baroni	SISSA		Watching flowers through a silicon glass: multiscale simulation of the color optical properties of natural dyes -- Topological quantisation and gauge invariance of charge transport in liquid insulators
European Researchers Night	27/09/2019	Trieste (IT)	Federico Grasselli Maria Celeste Maschio	SISSA CNR Nano		
Nanoscience and Nanotechnology - international meetings	15/10-18/10/2019	Frascati (IT)	Daniele Varsano	CNR Nano		
Beilstein Open Science Symposium 2019	15/10/2019	Rüdesheim am Rhein (DE)	Giovanni Pizzi	EPFL	Giovanni Pizzi	Open Science Platform for Materials Science: AiiDA and Materials Cloud

20th Symposium on Condensed Matter Physics	7-11/10/2019	Belgrade (Serbia)	Stefano Baroni	SISSA		Topological quantisation and gauge invariance of charge transport in liquid insulators
Grenoble-Barcelona twin conference : From quantum systems to new materials and smart electrical energy	23-25/10/2019	Grenoble (FR)	Zeila Zanolli	ICN2	Zeila Zanolli	Ab initio exciton and phonon dynamics in Transition Metal Dichalcogenides
Italy-Israel Workshop on 2D materials	26/11/2019	Israel	Deborah Prezzi	CNR Nano		
2D Materials, topological insulators and beyond	28-29/11/2019	Santiago de Chile (CL)	Zeila Zanolli	ICN2	Zeila Zanolli	Spintronics at the interface
Symposium: Computational and Theoretical Condensed Matter Physics	17-18/12/2019	Namur (BE)	Zeila Zanolli	ICN2	Zeila Zanolli	Spintronics at the interface
AiiDA Coding Week	09-13/12/2019	Fiesch (CH)	Giovanni Pizzi Francisco Ramirez & all other AiiDA developers	EPFL		
Workshop on Writing reproducible workflows for computational materials science using AiiDA	19-20 Dec 2019	Tokyo (Japan) @ ISSP	AiiDA developers	EPFL	AiiDA support	
EMA 2020	22-24/01/2020	Orlando (FL)	Francisco Ramirez	EPFL		Open Science Platform for Materials Informatics: AiiDA and Materials Cloud
QE Developers meeting 2020	16/01/2020	Trieste (IT)	Stefano Baroni Pietro Delugas Paolo Giannozzi Andrea Ferretti Pietro Bonfà Carlo Cavazzoni Fabio Affinito Ivan Girotto	SISSA CNR Nano and IOM CINECA ICTP		
MolSim-2020: Understanding Molecular Simulations	17/01/2020	Amsterdam (NL)	Nicola Marzari	EPFL	Nicola Marzari	The great acceleration in materials discovery
Invited talk @ Department of Chemistry of University of Cambridge	12/02/2020	University of Cambridge (UK)	Stefano Baroni	SISSA		Quantum topological effects in the transport properties of ionic conductors
Seminar @ University of Princeton	14/02/2020	Princeton (USA)	Daniele Varsano	CNR Nano		

CMD 20202 GEFES	31/08-4/09/2020	online	Stefano Baroni Elisa Molinari (advisory Board)	SISSA CNR Nano	Stefano Baroni	Quantum topological effects on the transport properties
GTC Conference	5-9/10/2020	online	Elisa Molinari Andrea Ferretti	CNR Nano		MaX and GPU
IndTech2020	27/10/2020	online	Giovanni Pizzi	EPFL	Giovanni Pizzi	Simulations and digital infrastructures to accelerate materials discovery.
CODES@OEHI #2 Virtual Hackathon	03-05/11/2020	online	Fabrizio Magugliani Conrad Hillairet Pietro Delugas Dirk Pleiter	E4 Arm, Juelich		
MARVEL distinguished lecture @EPFL	17/11/2020	online	Stefano Baroni	SISSA	Stefano Baroni	Gauge invariance of heat and charge transport coefficients in electronic insulators

CATEGORY 3: OTHER events (not defined in D9.1 point 2.4) - **[POLICY]**

Event Name	**Date (dd/mm/yyyy)**	**Where (City, Country)**	**Participant Name**	**Node**	**Speaker**	**title of the talk/poster**
MaX Kick-Off meeting	13-14/12/2018	Modena (IT)	All MaX members	MaX consortium		
BIG MAP consortium workshop	18/01/2019	Copenhagen (DK)	Elisa Molinari	CNR Nano		
Kick-Off meeting INTERSECT	05/02/2019	Modena (IT)	Elisa Molinari	CNR Nano		
FocusCoE Workshop	21/02/2019	Frankfurt (DE)	Elisa Molinari Luisa Neri	CNR Nano		
EuroHPC RIAG meetings	2019 and 2020	Brussels (BE)	Elisa Molinari	CNR Nano		
CECAM Brainstorming meeting: data driven initiative	25-26/03/2019	Lausanne (CH) @ CECAM	Giovanni Pizzi Thierry Deutsch Carlo Cavazzoni Fabio Affinito Pablo Ordejon	EPFL CEA CINECA ICN2		
EOSC-hub Week 2019	9-12/04/2019	Prague (CZ)	Giovanni Pizzi	EPFL	Giovanni Pizzi	Pathways for EOSC-hub and MaX collaboration
H2020 Programme Committee NMBP	08-09/04/2019	Brussels (BE)	Elisa Molinari	CNR Nano		

EMMC expert meeting on business aspects of materials modelling marketplaces	07/05/2019	Lausanne (CH)	Nicola Marzari	EPFL		
EMMC-CSA Workshop on Industrial impact of materials modelling – achievements and perspectives	8-10/07/2019	Torino (IT)	Elisa Molinari	CNR Nano	Elisa Molinari	Designing materials with HPC: the MaX European Centre
Digital Excellence Forum @ICT Proposers' Day	19-20/09/2019	Helsinki (FI)	Elisa Molinari	CNR Nano		
MaX-Graphene Flagship joint event @ Graphene Week 2019	23-27/09/2019	Helsinki (FI)	Elisa Molinari Nicola Marzari	CNR Nano EPFL	Elisa Molinari	Talk 1:European HPC initiatives and 2D materials research: collaborating and funding opportunities; Talk 2: HPC for 2D materials research
European HPC training stakeholder workshop	08/10/2019	Brussels (BE)	Daniele Varsano Maria Celeste Maschio	CNR Nano		
Kick-Off Meeting for "Materials and Molecular Modelling Exascale Design and Development Working Group"	11/05/2020	online	Andrea Ferretti	CNR		

CATEGORY 3: OTHER events (not defined in D9.1 point 2.4) - **[TRAINING]**

Event Name	**Date (dd/mm/yyyy)**	**Where (City, Country)**	**Participant Name**	**Node**	**Speaker**	**title of the talk/poster**
AiiDA plugins migration workshop	25/03/2019	Lausanne (CH)	Sebastiaan P. Huber Oscar Arbelaez Leopold Talirz Giovanni Pizzi & code developers	EPFL		
MaX Webinar: Arm SVE and tools for Hardware-Software co-design	16 & 18/04/2019	online		ARM	Filippo Spiga	
AiiDA - Tutorial on Writing Reproducible Workflows for Computational Materials Science	21-24/05/2019	Lausanne (CH)	Giovanni Pizzi Oscar Arbelaez & AiiDA developers Andrea Ferretti Alberto Garcia	EPFL CNR Nano ICMAB-CSIC		
High Performance Computing ELCoREL Workshop	3-5/06/2019	Altafulla (ES)	Miguel Pruneda	ICN2		

One day Blender Course @ Modena (IT)	27/06/2019	Modena (IT)	Daniele Varsano	CNR		
Eastern Africa School on Electronic Structure Methods and Applications	July 2019	Addis Abeba	Nicola Marzari Giovanni Pizzi	EPFL		
MaX Webinar: Industry and Materials Design at the eXascale: bridging the gap	04/09/2019	online		CNR Nano SISSA CINECA ICN2 EPFL Trust-IT		
Picking flowers: Hands-on FLEUR	09-13/09/2019	Juelich (DE) @ CECAM	Daniel Wortmann Stephan Bluegel	JUELICH		
Summer School on Advanced Materials and Molecular Modelling with Quantum ESPRESSO	16-20/09/2019	Ljubljana (SI)	Giovanni Pizzi Stefano Baroni Paolo Giannozzi Pietro Delugas	EPFL SISSA CNR IOM		
VASP and AiiDA Workshop	23-27/09/2019	Oslo (Norway)	Sebastiaan Huber	EPFL		
1ST TUMIEE Training School	23/09 - 04/10/2019	Crete (GR)	Davide Sangalli	CNR ISM		
Hands-on course on Computational Laboratory of Quantum Mechanics	23/10-17/12 2019	Modena	Daniele Varsano Andrea Ferretti	CNR Nano		
SISSA/ICTP Master in HPC (MHPC)	2019/2020	Trieste (IT)	Stefano De Gironcoli Ivan Girotto Ralph Gebauer	SISSA ICTP		
RWTH Aachen University Master Plan (contribution)	2019/2020 winter semester	Aachen (DE)	Stefan Bluegel Gregor Michalicek	Juelich		
Course on Atomistic and Quantum Simulation of Materials at EPFL	2019/2020 spring semester		Nicola Marzari Francisco Ramirez	EPFL		
CODES@OEHI Hackathon	28-29/10/2019	Bologna (IT)	Fabrizio Magugliani Dirk Pleiter	E4 Juelich		
1st Central African School on Electronic Structure Methods and Applications (CASESMA)	18-23/11/2019	Dschang, Cameroon	Andrea Marini Nicola Marzari Giovanni Pizzi	CNR Nano EPFL		

MaX Hackathon: Domain Specific Libraries for Material Modelling	25-29/11/2019	Trieste (IT)	Stefano De Gironcoli, Pietro Delugas, Ivan Girotto + Andrea Ferretti and many other MaX developers from CNR	SISSA, ICTP, CNR		
Computational School on Electronic Excitations in Novel Materials Using the Yambo Code	27-31/01/2020	Trieste (IT)	Stefano Baroni Andrea Ferretti Andrea Marini Daniele Varsano Davide Sangalli	CNR Nano and ISM SISSA		
CECAM workshop: Integration of ESL modules into electronic-structure codes	17-18/02/2020	Lausanne (CH)	Alberto Garcia	ICN2-CSIC	Alberto Garcia	The libgridxc and libpsml libraries: current status and perspectives
Hackathon on plugin and workflow development for AiiDA	17-21/02/2020	Bologna (IT)	Alberto Garcia Emanuele Bosoni Nicola Spallanzani Miki Bonacci Pietro Bonfà AiiDA developers	ICN2-CSIC, CNR Nano, EPFL	AiiDA developers	
Wannier90 v3.0 School - Virtual Edition 2020	25-27/03/2020	online	Giovanni Pizzi	EPFL	Giovanni Pizzi	Automated high-throughput Wannierisation
ETSF's Top Online Tutorials	April 2020	online	Stefaan Cottenier Daniele Varsano Zeila Zanolli	UGent CNR Nano ICN2	Stefaan Cottenier	online course on Computational Materials Physics
Digital Learning after its Black Swan	28/04/2020	online	Stefaan Cottenier	UGent		
Fireside chats for lockdown times: a gentle introduction to density-functional theory	15-17/04/2020	online	Nicola Marzari	EPFL	Nicola Marzari	Density-functional theory Density-functional practice Applications and limitations
MaX webinar series on Flagship Codes	From 13/05 to 12/11/2020	online	MaX Consortium			
AiiDA Tutorial Week	7-10/07/2020	online	Giovanni Pizzi Marnick Bercx Francisco Ramirez Miki Bonacci Emanuele Bosoni & AiiDA developers	EPFL CNR Nano ICN2		

CATEGORY 3: OTHER events (not defined in D9.1 point 2.4) - [OUTREACH]

Event Name	Date (dd/mm/yyyy)	Where (City, Country)	Participant Name	Node	Speaker	title of the talk/poster
CECAM workshop: Extended Software Development Workshop: Scaling Electronic Structure Applications	07-09/01/2019	Dublin (IRL)	Alberto Garcia	ICN2-CSIC	Alberto Garcia	Status of GridXC
Novel Materials to rethink the world @ Uniud	08/01/2019	Udine (IT)	Nicola Marzari	EPFL	Nicola Marzari	
Materials and Scientists of the Future: the Space Girls visiting MaX CoE	05/03/2019	Modena (IT) @ MaX CoE	Elisa Molinari	CNR Nano		
Seminar @UniPR	10/05/2019	Parma (IT)	Fabrizio Magugliani	E4		
SMAU - Research to Business	06/06/2019	Bologna (IT)	Luisa Neri Elisa Molinari Maria Celeste Maschio	CNR Nano		
35th International CAE Conference	28-29/10/2019	Vicenza (IT)	Fabrizio Magugliani	E4		
EPFL Open Science Day	18/10/2019	Lausanne (CH)	Nicola Marzari	EPFL	Nicola Marzari	Project Snow White
The importance of being H.P.C. Earnest	18/06/2020	online	Nicola Marzari	EPFL	Nicola Marzari	The great mysteries of computational science, and the marvelous opportunities
ESOF 2020	2-6/09/2020	Trieste (IT) + online	Elisa Molinari	CNR	Elisa Molinari	
Swiss Research Data Day 2020	22/10/2020	online	Francisco Ramirez,	EPFL	Francisco Ramirez	AiiDA 1.0, a scalable computational infrastructure for automated reproducible workflows and data provenance
European Researchers' Night	27/11/2020	online	Maria Celeste Maschio Claudia Cardoso Nicola Spallanzani	CNR		

CAE Conference	30/11 - 4/12/2020	online	Fabio Affinito Fabrizio Magugliani Alberto Garcia Maria Celeste Maschio Luisa Neri Francesco Osimanti	CINECA E4 ICN2/CSIC CNR Nano Trust-IT		