



## D9.1

# MaX Communication and Dissemination Strategy & Stakeholder Engagement Plan

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Deliverable D9.1  
 MaX Communication and Dissemination Strategy &  
 Stakeholder Engagement Plan

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## D9.1 MaX Communication and Dissemination Strategy & Stakeholder Engagement Plan

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## Executive Summary

The main goal of MaX (Materials design to the exascale)<sup>1</sup> is to allow the pre-exascale and exascale computers expected in Europe in the 2020's to meet the demands from a large and growing base of researchers committed to materials discovery and design. All this is made possible by the coordinated effort of a team involving developers of the leading EU open source community codes in the materials domain, five leading European HPC centres, two technology partners, and training and communication experts.

In line with this goal, this document sets out a strategy for communication and dissemination. Both, communication activities, as well as dissemination activities, contribute fundamentally to ensure a coordinated and continued communication of the MaX project, providing appropriate visibility to all stakeholders. Deliver and maintain an actionable communication plan with feasible KPIs, describing all global, outreach activities that are going to be performed to support stakeholders (& new ones from the call) and their engagement.<sup>2</sup>

This document will provide guidance to the projects' partners in order to make the most of their activities reaching various target groups. This strategy document outlines the main objectives, target groups, tools and activities for communication and dissemination of the MaX.

The MaX communication strategy is a SMART (specific, measurable, achievable, relevant, and time-bound) and KPI-driven approach to successful community building and stakeholder engagement, design and promotion of the MaX events, content creation and development of the Communication toolbox and social media campaigns. Moreover, experience has demonstrated, amongst many things, that the most important Dissemination



recommendations and actions should be Realistic, Implementable, Achievable and Measurable.



## Abbreviations and Acronyms

|                  |  |
|------------------|--|
| ACS              | - American Chemical Societies  |
| AiiDA            | - Automated Interactive Infrastructure and Database for computational science                    |
| APS              | - American Physical Societies  |
| BSC              | - Barcelona Supercomputing Centre / Centro Nacional de Supercomputación                          |
| CEA              | - Commissariat à l'Énergie Atomique et aux Énergies Alternatives                                 |
| CECAM            | - Centre Européen de Calcul Atomique et Moléculaire  |
| CIN/CINECA       | - Consorzio Interuniversitario Cineca  |
| CNR              | - Consiglio Nazionale delle Ricerche   |
| CoE              | - Center of Excellence   |
| CSA              | - Coordination Support Action  |
| CSCS             | - Swiss National Supercomputing Centre   |
| D8.1             | - MaX Training and Education Programme   |
| D9.1             | - MaX Communication and Dissemination Strategy & Stakeholder Engagement Plan                     |
| EOSC             | - European Open Science Cloud  |
| EPFL             | - Ecole Polytechnique Fédérale de Lausanne   |
| ETHZ             | - Eidgenössische Technische Hochschule Zürich  |
| EU               | - European Union   |
| EMMC             | - The European Materials Modelling Council   |
| FLEUR            | - Full-potential Linearised augmented plane wave in EUROpe                                       |
| 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   |
| MaX-E            | - MaX event  |
| MaX-T            | - MaX training event   |
| MaX-C            | - MaX community/EuroHPC event with MaX participation   |
| MRS              | - Materials Research Society   |
| QUANTUM ESPRESSO | - Quantum opEn-Source Package for Research in Electronic Structure, Simulation, and Optimisation |
| SISSA            | - Scuola Internazionale Superiore di Studi Avanzati, Trieste                                     |
| SME              | - Small Medium Enterprise  |
| SW               | - Software   |
| UZH              | - University of Zurich   |



WP - Work Package

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## 1 Introduction

### 1.1 Purpose and scope

MaX's first major goal is to enable 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. MaX will also enable high-throughput computing, with a huge number of simultaneous simulations on pre-exascale machines, will provide HPC- and HTC enabled software and concepts to the broad community of code developers, will support the convergence with high-performance data analytics, will foster the creation of a broad and skilled talent pool in Europe, and ultimately will boost the use of HPC and HTC in industry and academia.

With the approach adopted and a strong orientation to co-design, MaX will pave the way for the transition to and beyond exascale technologies. MaX will adopt a sustainable software development strategy to cope with the abrupt technological disruptions to be expected in the years to come, whereby exascale ready software solutions will be easily ported and shared across different codes, thus realising a substantial economies of scale, and shortening the time needed to adapt to a rapidly evolving technology.

The purpose of the present document is to define the strategy and plan and foreseen activities for communication and dissemination for MaX WP9, "MaX Communication and Dissemination Strategy & Stakeholder Engagement Plan". In particular, a drill-down on the stakeholder groups and channels utilised is also enclosed and the mechanisms, tools and procedures the consortium is putting into place to help deliver this second phase of the project into a more **impact driven activity**, and where the recommendations from MaX first phase have been considered - especially towards a strategy to support onboarding: A ) Industry; B) The General Public & Civil Society & C) Better European engagement in general.

The deliverable defines the different types of stakeholders, the engagement strategy devised for each of them, and the procedures and tools to be employed to ensure a **streamlined, continuous** running of the engagement activities. These include the communication activities which will facilitate the outreach of the target research communities at key events.

Clearly, owing to the early stage in the project, some of the detailed information around results achieved and communication and dissemination assets related to those still not available at the time of writing. Therefore, the report is effective to be considered, for some aspects, as a "living document", which will not be changed in the core structure, but could be updated or expanded (for instance with guidance documents in the Annex).



## 1.2 MaX Communications as a result of MaX first phase

The overall effort of MaX first phase has been focused around several communication goals:

1. to develop a unified and coherent MaX image which sees also the branding of products and services;
2. to communicate in an easy manner MaX strategy, goals and early achievements;
3. to enhance community identity among MaX stakeholders;
4. to promote MaX services, especially those industry-oriented services;
5. to communicate major MaX achievements and success cases to the specialized and general audiences.
6. to highlight the strategic and related co-operations taking place in and around Europe that support both the training as well as the communications strategies in place.

We have also positioned the communication strategy to prepare MaX for the future Centres of Excellence (CoE) evolution. The extensive amount of work, services offered, results of research have been conveyed to different specialized communities (including: code developers and users, HPC world, stakeholders plus institutional and political actors) and the general public by a different number of channels. Following the review recommendations, from the first phase of MaX [2015-2018] we have made a concerted effort of thinking and adapting of tailoring our messages around the stakeholder we are dealing with in order in order to back up the engagement to the public, and we have especially focused on engaging a broader audience on both the results of MaX activities and its contribution to the European HPC environment.

Concerning the **general public**, the main actions and channels involved included:

- **Social media channels:** great part of general-content communication has been done through Twitter account (@max\_center2) and, at a lesser extent, through the LinkedIn account. Social communication aimed at promoting CoE life and its activities out of lab. Moreover, there was an effort to participate to the stream of social communication, and contents were provided or just shared to promote ideas and information about the surrounding social and cultural environment, about general science, materials and HPC basic concepts, events. The CoE's strong interest in gender issues was communicated with the writing or sharing of 24 gender-specific tweets.
- **Institutional website entry page** ([www.max-centre.eu](http://www.max-centre.eu)): we tried to convey some general-public concept by focussing on MaX's results presented through visual and text, in order to offer to the website visitors the chance of getting at first glance what MaX was doing.
- **Events for the general public:** MaX researchers participated to several public events, that were timely presented in our communication channel. Among the others, we mention:



1. Participation to the 2017 European Researchers' Night in Modena (CNR NANO) on September 29, 2018.
2. Professor Nicola Marzari presentation "New materials to rethink the world" in Teatro Piccolo Eliseo in Rome, for the "Science Mondays" Festival.
3. Radio show: Elisa Molinari was the guest of a radio interview in two parts about "Time to reach exascale", on air on Radio24, an Italian national all-news radio station.

Concerning the **more specialized public of code developers and users**, which are the main users of the CoE and the community, the consortium wanted to fully engage, the main actions and channels involved included:

- MaX newsletter: drafting, editing and implementation of 4 issues of the newsletter (20/04/2017; 08/08/2017; 24/11/2017; 13/07/2018).
- Institutional website with continuous updating with institutional information about the CoE and all WP activities, news & events, documents related to the CoE life.
- News about the CoEs activities were diffused through different channels in order to achieve the highest impact, especially when promoting/reporting training and dissemination events.
- Cross-activities with flagship codes: crosslinks between website plus a strategy of retweeting and pushing news from codes' or MaX's social media accounts was used, in order to take advantage of the social media multiplier effect. This has happened especially with Quantum Espresso (@quantumESPRESSO) and Aiida (@aiidateam).

Concerning **the specialized public of HPC world**, the main actions and channels involved included:

- MaX newsletter: several news in the Newsletter were targeted to HPC-specialists, to inform them about MaX-related activities of their interest.
- Social media: several tweets, original or shared, on HPC issues and events, often linking to other sources (e.g. using #HPC, #EuroHPC). Several tweets connect to flagship codes.

Concerning the dissemination of the MaX activities and objectives to its stakeholders, including institutional and political actors: MaX was committed to actively engage stakeholders, as different as they can be. In order to do this, several actions were undertaken at dissemination level, several in communication actions.

- Social media: continuous interactions with several institutions at national and European level (sharing of contents or news diffusion); use of #EuSciComm, #eInfraEU; co-sharing of contents with other CoEs accounts and other projects' accounts; promotion of MaX activities towards HPC organizations and co-sharing of contents (e.g. with PRACE, Psi-k accounts);
- MaX organized/participated in several meetings with institutional and political representatives at a National and Regional level, and with high-level managers of national research/industry/higher education organizations. In the communication at/around the meetings, our emphasis has been on presenting on one side MaX, its impact and perspectives, on the other side the relevance and potential of the whole



European strategy on HPC towards the exascale, with a key role for materials science applications. Generally speaking, the feedback was very positive, and in some cases it led to commitments in terms of support to MaX and to European HPC policies, both of relevances for medium or long term perspective sustainability of MaX.

Some useful statistics:

- Website ([www.max-centre.eu](http://www.max-centre.eu)): total visitors 103.101; total visits 284.469;
- Twitter account (@max\_center2): 435 followers;
- The MaX periodic newsletter: 745 subscribers.

### 1.3 Structure of the document

The **MaX Overall Communication and Dissemination Strategy & Stakeholder Engagement Plan** is part of the endeavours of WP9 ("Engagement, Communication, Dissemination & Uptake"). Given the cross-cutting theme of the WP, the ideas and guidelines sketched out in this document affect the creation of all content within the project. All organizations involved in the project are expected to contribute to communication, dissemination and impact. They are asked to follow the communication guidelines, which will be provided in this document and through other means (templates, etc.).

While all WPs engage in communication, there is a strong connection to specific WPs, which are dedicated to leveraging on state-of-the-art communication activities to effectively engage with the MaX stakeholders (WP8 "Training and User Uptake") and the creation of the project's infrastructure (WP5 "Ecosystem for HPC, HTC and HPDA convergence"). Specific actions, which are also affected by this plan, are:

- MaX web platform (WP5, WP8)
- Communities engagement (WP8, WP9)
- D10.1 First report on CoE governing bodies, KPI, and infrastructure setting up
- Continuous communication and dissemination of MaX research and innovation activities (all WPs)

The document is organised in three central sections:

- Section 2 defines the project strategy for stakeholder engagement. Objectives, stakeholders, value propositions and channels are explained in detail.
- The assets available for dissemination and communication, arising from the expected project results, are described in Section 3.
- Section 4 lays out the Communication and Dissemination plan itself.

## 2. Strategy



MaX is innovative, forward-looking, and important to different stakeholders. Efficient communication contributes enormously to its success and contributes to maximizing the project's reach. Thus, the main objective of this document is to ensure the effectiveness of the communication and dissemination activities to widely promote the innovation and benefits of MaX to targeted stakeholders, maximize visibility, activate end-user communities, disseminate results, and demonstrate impact. It is an overall communication objective that the project's output. All partners will contribute to the concerted efforts, including joint collaborative actions with peer projects and the funded CSA, and with specialists within the consortium contributing to relevant standardisation and frameworks.

The different partners from different WPs will need to input and access information related to the stakeholder communities and engagement activities carried out. Particularly for the training and workshop, WP8 will be work hand-in-hand with to collect all the organized and co-organized events, trainings and workshops relevant for MaX. The participation of different persons in the interactions with the communities might generate a confused message to the stakeholders as well as an increased risk for some stakeholders not to be properly considered.

For this reason, WP9 put into place an online shared system to keep track of the different stakeholders and the actions taken towards each community group together with the indication on who is responsible for updating which part of the system. The general approach will be that whenever a MaX partner team member is in contact already with the community, he/she will be responsible for the specific engagement with the community; for new communities (not in contact already with any MaX partner) will be assigned to one of the task 9.2 team members in coordination with WP8.

The collection and update of information on the stakeholder engagement involves in particular to:

- Define, and implement a database of all the stakeholders relevant for the MaX project;
- Fill in the database with the initially identified communities with which MaX partners are already in contact;
- Identify who is in charge to act as maintain main contact with the stakeholder and to keep the information on the database up-to-date;
- Maintain the database along the project lifetime;
- Trigger other WPs as needed.

A first structure for the database of stakeholders has been identified and it contains: (see Annex II)

- Type of stakeholders: stakeholders to allow targeted communication or messages to be created. The type of stakeholder can be selected from the list used in the table 1;
- Community: name of the community/stakeholder;
- Description: short description of the community;
- Disciplinary area: main scientific domain for the community;



- Main contact within the entity: reference person for the community;
- Role: identify the role of the contact within the community;
- Owner in the project: who within MaX team is responsible for the engagement with the community;
- Priority: priority in the engagement which will be decided based on the level of influence, power, and interest;
- Why to engage with them: which is the main reason and objective of the engagement with the specific community;
- Channel to reach them: best channel to be used to reach the expected engagement as described in detail in section 2.4.

In addition to stakeholder database, WP9 puts into place an online shared system to consolidate all the MaX Services, Results & Assets and the 3 questionnaires to each WP leader to generate the detailed information about each MaX flagship code based on the first phase of the project.

The 3 questions have been identified and share to the MaX flagship code leaders are: (see Annex II)

Q1: Does your result meet any specific need of any specific end-user with this innovation?

Q2: Why is your solution better than any other existing one on the market?

Q3: What is the societal benefit - is your result also a social innovation and if yes explain how this is the case?

A first structure for the database of MaX Services, Results & Assets has been identified and it contains: (see Annex II)

- WP Number: number of the WP
- WP Name: name of the WP
- WP Leader: who within MaX team is responsible for the WP
- Partner: the organization of the WP leaders
- Products/Services: indicate the particular products and services of the organization
- Code: the MaX flagship code assign on the WP
- Code description: the short and concise description of code
- Code Leader: who within MaX team is responsible for the MaX flagship code
- Demonstration: indicate the particular demonstration that the Code will performed
- Software (SW) Applications): identify the SW application generated within particular code
- Tools: identify the developed tools within particular code
- User Support: specify the user support activity provided by the code
- Quantum as a Service:
- Platform: identify the platform used within particular code
- Training: identify the training/s provided within particular code
- Exascale: identify the activity within the code that leads to exascale

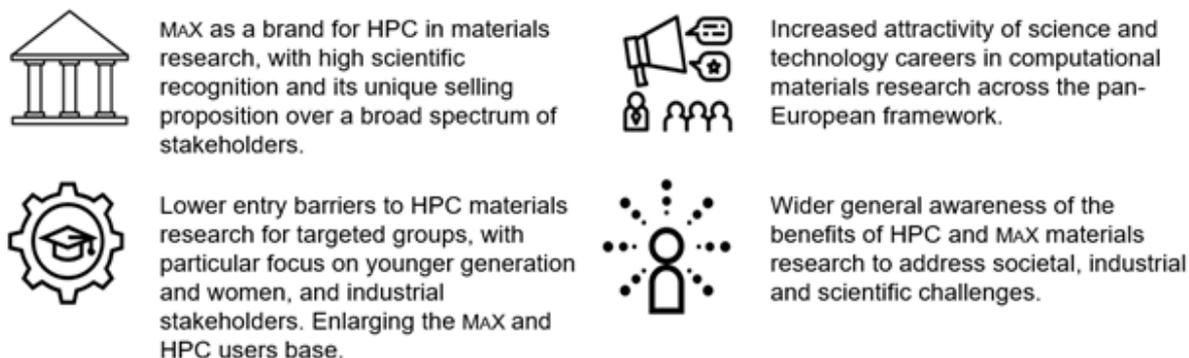
- SW Architecture 129 Data Stewardship: identify the activity within the code that leads to SW Architecture 129 Data Stewardship
- Main Output of the Code Centre: identify the main output of the code from the first phase of the project

To ensure coordinated, regular communication of MaX, providing the opportunity of visibility to all stakeholders, as well as developing an effective exploitation approach and sustainability, the following strategic elements have been established, in good agreement with the provisions of the grant agreement.

## 2.1 Objectives

MaX aims at providing an open-access infrastructure with benefits to different target groups. The intended main impacts of the communication actions are:

Figure 1: MaX communication: impacts



The above impacts will be achieved through a set of communication and dissemination activities including:

- 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
  - Videos
  - In-house newsletters
  - Press releases



- o Posters
- Delivering a communication strategy, with measurable targets, to motivate continuous activities and measure impact, including, but not limited to:
  - o Community development
  - o Web analytics
  - o Social media analytics
  - o Community database profiling
- Producing high-quality and highly relevant content for the MaX web platform, LinkedIn and Twitter. Creating media content on major achievements and insights on developments.

## 2.2 Stakeholders

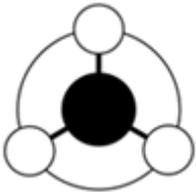
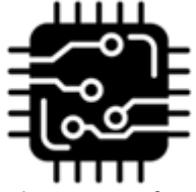
In order to perform an effective communication towards the most identified Stakeholders, a seamless synergy with WP8 “Training & Uptake” will be put in place. Engagement will be measured by means of stakeholders that contribute to the various activities in place, stakeholders who attend meetings or other physical or virtual events with an adequate level of identification, social media channel followers. The results will be captured in the deliverables. The central scope of the task directly translates into establishing a continuous dialogue with all the stakeholders selected, also with the support of an effective and pragmatic engagement plan. Actions will target the 7 major stakeholder groups identified in Table 2), which provide a thorough range of actors, and have received letters of support/commitment from the majority of the stakeholders (MaX grant agreement Sec. B.2.2).

**Table 1. MaX Priority Stakeholders**

| Priority Stakeholder Group  | Main outcomes of interest   | Dissemination vehicles   |
|---|---|--|
|  <p>1. European and member states institutions</p> | <ul style="list-style-type: none"> <li>● Pre-exascale and exascale computing capabilities. Scalable and sustainable parallel codes (wider use across science, industry and to address societal challenges).</li> <li>● Sustainability Plan. Less fragmentation across member states through collaboration.</li> </ul> | <ul style="list-style-type: none"> <li>● Online reports</li> <li>● Policy recommendations, MaX plans and roadmaps</li> </ul> |



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|  <p>2. European HPC ecosystem<br/>         (EuroHPC, HPC centres, Prace,<br/>         ...)</p> | <ul style="list-style-type: none"> <li>Codes portable to &amp; scalable on future HPC computing platforms.</li> <li>Joint contributions to the EuroHPC strategy.</li> <li>Contributions to joint training initiatives. Avoided duplication and increased impacts.</li> </ul>   | <ul style="list-style-type: none"> <li>Joint promotion on common goals, training, technical and results showcase events. Common approaches</li> </ul>   |
|  <p>3. Hardware Manufacturers</p>  | <ul style="list-style-type: none"> <li>Shared co-design cycle and strategies for the design of new products. Demonstrated new benchmarks, e.g. performance, energy efficiency, scalability.</li> </ul>   | <ul style="list-style-type: none"> <li>Co-design reports.</li> <li>Roadmaps and SW/Data plans.</li> <li>Technical reports.</li> </ul>   |
|  <p>4. Industrial &amp; academic end-users</p>  | <ul style="list-style-type: none"> <li>Flagship codes ready for use on pre-exa architectures, and prepared for the evolution to exascale. User-friendly adoption packages and documentation for HPC &amp; HTC. Easy access to research data, SW, reports.</li> <li>User-oriented workflows and turn-key solutions with potential for bespoke support.</li> </ul> | <ul style="list-style-type: none"> <li>Collaboration with FocusCoE for targeted outreach activities (e.g. sectorial industrial events). and dedicated info packs.</li> <li>Downloadable SW &amp; documentation. Dedicated technical workshops, hands-on training/hackathons/summer schools with online re-usable content for self-paced skills development.</li> <li>Individual code forum, mailing lists.</li> </ul> |
|  <p>5. Independent software vendors (ISVs), code developers</p>                              | <ul style="list-style-type: none"> <li>Codes, modules, libraries, where code modularisation -- central to the MaX strategy-- is a key ISV asset. Extended in-code documentation.</li> </ul>  | <ul style="list-style-type: none"> <li>Downloadable SW &amp; documentation.</li> <li>Individual code forum, mailing lists.</li> <li>Dedicated training events and re-usable materials.</li> <li>Briefings/1-2-1 meetings at events</li> </ul>   |

|   |  |   |
|---|--|---|
|  <p>6. Large scale experimental facilities</p> | <ul style="list-style-type: none"> <li>• Containerisation for easy use of codes by experimental teams.</li> <li>• Integrated data strategies, moving codes to data. New benchmarks.</li> </ul>   | <ul style="list-style-type: none"> <li>• Downloadable SW &amp; documentation. Dedicated technical workshops, hands-on training and online re-usable content.</li> </ul>   |
|  <p>7. Education system</p>                    | <ul style="list-style-type: none"> <li>• Education and teaching materials (undergrad and graduate students level) including hands-on modules based on open source codes</li> <li>• On-line training modules for self-paced learning</li> </ul> | <ul style="list-style-type: none"> <li>• Teaching and training events; material to suit different needs.</li> <li>• Ready-to-use workflows.</li> <li>• Easy access to open source codes and documentation. Quantum Mobile virtual machine.</li> </ul> |

### 2.3 MaX Value Proposition

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.

Figure2: MaX Value Proposition





## 2.4 Channels

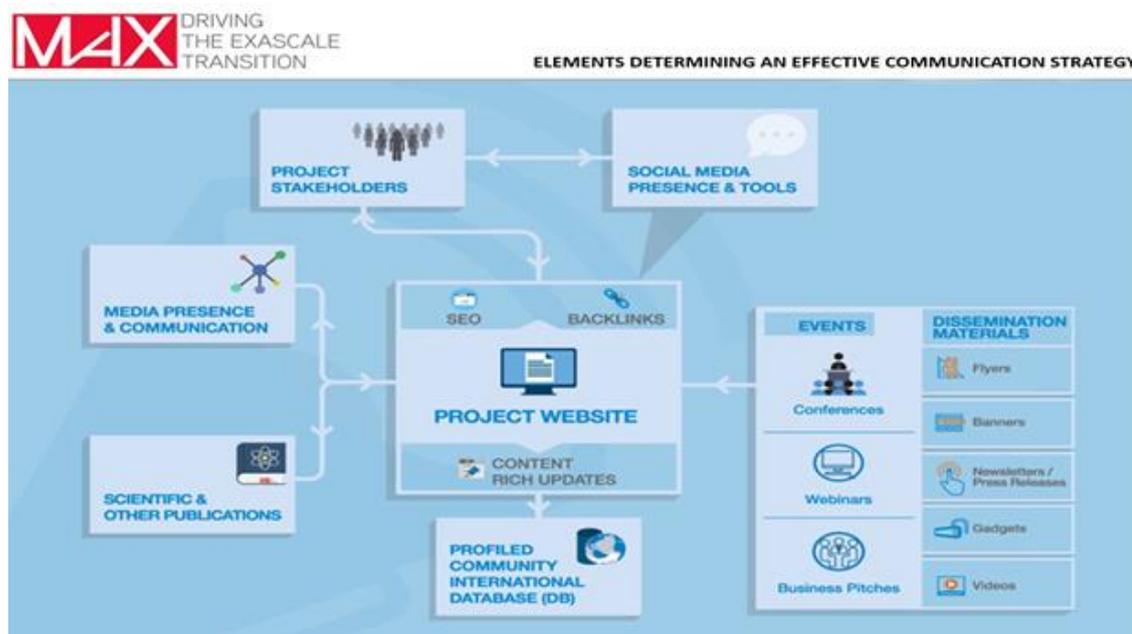
MaX will use various communication channels, leveraging in part on the project partner networks, and will produce a set of tailored communication formats targeting different stakeholder groups. The consortium can count on extensive expertise and experience in creating a communication kit with diverse formats and extend the strong network by reaching out to a broad range of stakeholders, media, professional and social channels. The main channels that will be utilised in MaX are visualized in Table 2 together with the affinity of the stakeholder groups to these channels.

Figure 3, which has been taken from the description of the strategy delivered by Trust-IT on the pilot project issued by the EC in 2017 – entitled the Common Dissemination Booster, supporting European Commission projects cluster together to disseminate more effectively, describes the communication channels and the other elements at the basis of an effective communication strategy.

**Table 2: Heatmap indicating stakeholders, general public and their affinity to MaX communication channels**

| Channel                              | Assumed affinity of stakeholders to communication channels |  |                        |                                 |  |                                     |                  | Special Focus  |            |
|--------------------------------------|--|--|------------------------|---------------------------------|--|-------------------------------------|------------------|----------------|------------|
|                                      | European and member states institutions                    | European HPC ecosystem (HPC centres, Prace, Euclid, ...) | Hardware Manufacturers | Industrial & academic end-users | Independent software vendors (ISVs), code developers | Large scale experimental facilities | Education system | General Public |            |
| MaX Website                          | Light Blue   | Light Blue   | Dark Blue              | Dark Blue                       | Dark Blue  | Dark Blue                           | Dark Blue        | Dark Blue      | Dark Blue  |
| Social media                         | Dark Blue  | Dark Blue  | Light Blue             | Dark Blue                       | Light Blue   | Light Blue                          | Light Blue       | Light Blue     | Dark Blue  |
| Events (physical and virtual)        | Light Blue   | Dark Blue  | Light Blue             | Dark Blue                       | Dark Blue  | Dark Blue                           | Light Blue       | Light Blue     | Light Blue |
| Traditional media and other channels | Dark Blue  | Dark Blue  | Light Blue             | Dark Blue                       | Light Blue   | Light Blue                          | Dark Blue        | Dark Blue      | Dark Blue  |
| Video production                     | Dark Blue  | Dark Blue  | Light Blue             | Dark Blue                       | Light Blue   | Light Blue                          | Dark Blue        | Dark Blue      | Dark Blue  |

Figure 3: Elements determining an effective communication strategy



### Social media and professional networks

Social media is a core element of MaX communication, especially to follow ongoing developments and to connect to different stakeholders. MaX makes use of Social Media channels and professional networks such as Twitter, LinkedIn, YouTube in order to build a stronger and highly engaged MaX community. Additionally, the MaX Flagship codes will encompass community interaction through professional networks (e.g. code forum/ mailing list, Psi-k network) with the goal to enable contributions and successful uptake of any developments. .

### Events

To maximise impact towards MaX stakeholders and in collaboration with relevant WPs, such as WP5 and WP8, WP9 is promoting and supporting the organisation of EU-wide targeted workshops, coordination meetings, webinars, workshops, training events. There will be events organised by MaX, co-branded events of the institutions participating in MaX, MaX Community trainings and workshops, in which MaX will be present, and events co-organized with the European HPC ecosystem, e.g. FocusCoE and PRACE. The presence and active contributions of MaX partners at events (session, paper or poster, etc) will be mapped in a shared document to plan engagement and promotion effectively.

Examples of large events exclusively organized by MaX include the project kick-off and the MaX final conference. Beside these large events, which showcase the project's progress and achievements and engage with a broader range of stakeholders and other European initiatives, there will be a number of smaller MaX-dedicated events. Also



organized by MaX, together with the developers teams, are the large number of training activities described in D8.1.

3rd-party events include e.g. exhibitions and conferences on HPC and scientific conferences and meetings (EOSC Hub Week 2019, European HPC Summit Week 2019, PASC 2019, ISC 2019) where MaX CoE actively participates.

A special case is the collaboration with Psi-k, the community Network in electronic structure based calculations: MaX has agreed to co-fund a series of workshops for broader dissemination and community engagement. The main Psi-k conference, that takes place every 5 years and is planned for 2020 in Lausanne, will be the opportunity for selected joint MaX - Psi-k activities including a scientific session and two community sessions/events especially targeted to young people and women. Stakeholders 4 and 5 will especially benefit from these activities (as well as from training activities in collaboration with CECAM).

A special agreement was reached with the Graphene Flagship to jointly organize a scientific session within the Graphene week (Helsinki, September 2019) on frontiers of HPC for 2D materials research, as well a policy session on the opportunity of collaboration between the Flagship, MaX and European HPC initiatives in general.

MaX will leverage coordination with other CoEs and the FocusCoE especially for what concerns dissemination activities towards industry and SMEs. Indeed, the CoEs and FocusCoE have decided to focus their joint work plan on the coordinated participation in/organization of sectorial industry-oriented events. This joint effort, coordinated by FocusCoE, is expected to increase attractiveness and impact towards these stakeholders (sofar this was found to be a major challenge by all CoEs).

### **Publications and technical conferences**

MaX dedicates effort under WP9 to disseminate major results, that will be publicly available via peer-reviewed publications based on collaborative work undertaken within the project. Below we provide a sample of targeted scientific conferences and publications to validate and disseminate technology advances from MaX. Involved partners are indicated in square brackets, according to the categories defined in Table 1.

- Scientific conferences and workshops on HPC, targeting mostly the HPC community and HW stakeholders [HPC centres, technology partners], see e.g.: SC SuperComputing.
- 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], such as the ones organized by the Materials Research Society (MRS) in Europe and the US, the German Physical Society (DPG), the American Physical and Chemical Societies (APS, ACS), just to cite the ones with broader audience.
- Scientific Publications targeting the HPC community [HPC centres], e.g. IEEE Transactions on Parallel and Distributed Systems and IEEE Transactions on Industrial Informatics.
- Scientific Publications targeting end-users of materials simulations and code developers [codes & ecosystem developers], such as the journals of Nature Publishing



Group, American Physical and Chemical Societies, Royal Society of Chemistry, American Institute of Physics, Springer, Wiley and many others.

### Traditional media and other channels

Notwithstanding continual usage of web, social media, and visibility at specialised events, MaX will also dedicate effort to ensure presence in “traditional media” with the main goal of further expanding outreach, especially to large numbers of Research Centres, Academia, European SMEs and Citizens. A sample is provided below and includes channels with which the MaX consortium already has close links.

**Table 3: Sample of channels to reach MaX stakeholders**

| Stakeholder Group(s)  | Channels and Networks   |
|---|---|
| Domain-specific and scientific communities                    | CECAM and Psi-k as partner international scientific organisations scientific societies (e.g. Materials Research Society, National and European Physical Societies)  |
| Young people for training, education and career opportunities | ETSF (upcoming young researchers meeting); European Researcher Nights events; Psi-k network and its job opening advertising; Associations for Women in Science; Women in Tech and similar twitter accounts (partners are already active on 5 forums); Master and PhD programs involving partners (e.g. SISSA-ICTP 12-month Master Programme in HPC) |
| Developer/User communities                                    | Code community (forum, mailing list)  |
| LinkedIn Groups   | High Performance and Supercomputing (25K); High Performance Computing (24K); HPC Group (5K).  |

## 2.5 MaX Service Oriented Web Platform

Engagement with the general public will predominantly happen through the project Website (<http://www.max-centre.eu/>). This serves as the unique access point for the MaX Flagship Codes, Trainings and Services for the future of materials modelling and it will showcase the project’s objectives and partners, news, and events.

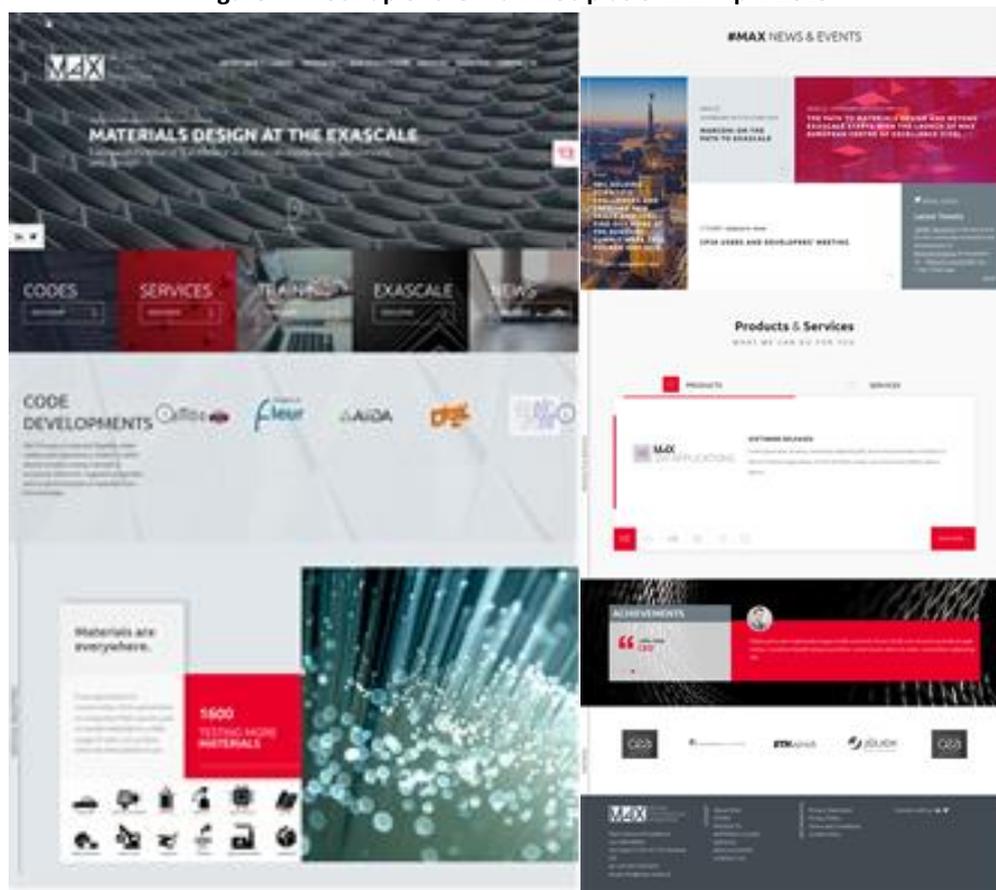
A preliminary version of the website was already up in month 1 at the start date of the project. The first version of the revised MaX’s website is being finalized (website revamp tailored to MaX as part of the tool kit element) providing information about the project and the MaX code suite, products, training and services. Users could register an account and receive the newsletter. The webpage is planned and structured to ensure visibility and easy access to the technologies and services, as well as innovations mechanisms in data production, use cases and training materials, targeting data producers, data users, and reusers in the MaX ecosystem as well as industry players.

The website will also serve as the main repository for all published content and allow access to project deliverables and external resources. It will have specific sections dedicated to events, news, trainings and services and it may contain sections for services that will provide basic and advanced support, quantum as a service and



helpdesk service. It will be able to host code development repositories developed within MaX Code suite and it will provide direct access points to the the MaX industry. The MaX website will have different iterations during the project’s lifetime aligned with the forthcoming results.

Figure 4: Mock up of the MaX web platform in April 2019



## 2.6 KPI-driven approach

This plan adopts a SMART approach to its continuous communication activities along the 36-month project life-cycle [specific, measurable (KPI-driven), achievable and realistic (based on identified target groups and channels to reach target groups), timely (matched to project opportunities and results) and timed (clear start and end date)]. KPIs that are relevant for communication and engagement are indicated in the table 4 “MaX Communication and Dissemination KPIs”. The roadmap clearly defines a set of macro activities which include more detailed, specific activities that the Consortium will undertake to ensure an effective communication and outreach strategy spanning across a 36-months period.



Evaluation of the communication and dissemination activities will be based on several reference points. The final version of the communication & dissemination strategy & stakeholder engagement plan in M24. Measurable impacts (KPIs) are tracked on a monthly basis through a “Flash Report” monitoring the visibility, engagement, and dissemination potential of online activities in an automated software which extracts, analyses, and visualises the selected KPIs (explained in section 5). There will be a preliminary report on impact assessment in M18 and a final report on impact assessment in M36. These deliverables will indicate the actions taken to engage stakeholders and the effectiveness of the communication and promotional campaigns. Two iterations are foreseen.

**KPI-based Communication Toolbox**

A professional and dynamically evolving Communication ToolKit will cover the design and maintenance of the communication toolkit elements. MaX will produce various communication formats tailored to the different stakeholder groups. These formats include content-rich approach tailored to MaX, community building through social media and professional networks, training videos from events, collateral and promotional materials, slideshare or presentation, press releases and media content, etc. These form part of the MaX communication toolkit as an essential part of the communications and dissemination strategy and stakeholder engagement plan. The strategy is KPI-based and includes joint actions of the other related work packages. A set of training presentations clustered by stakeholders and topics (and published for later use). The elements, related measures and metrics regarding communication and dissemination actions that the project will undertake to ensure the effectiveness of its outreach and impact assessment strategy are stated below in table 4.

**Table 4: MaX Communication and Dissemination KPIs**

|                          | <b>Toolkit element</b>  | <b>KPI (total numbers over 36 months)</b>   |
|--------------------------|---|---|
| Communication<br>Toolbox | Press releases  | min 1 press release or article/year for specialist press.<br>min 2 articles for the general public.   |
|                          | Print material (Flyers, posters, pop-up banners, infographics, brochures etc. tailored to different stakeholders and regularly updated to reflect project progress. ) | Min. 1 update every 6 months.<br>Min. 1 collaboration promotional pack/year.<br>Dedicated promotional packs for all events.<br>Flash report monitoring on core statistics |



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|                                      |                                      |  |
|--------------------------------------|--------------------------------------|--|
|                                      | Presentation (connected to LinkedIn) | All training presentations clustered by stakeholders and topics<br>All presentations from technical and showcase events<br>Min. 1 updated project slide deck/year.<br>Flash report monitoring on core statistics |
|                                      | Document templates                   | 1 template for internal and public deliverables<br>1 template for external communication   |
|                                      | Newsletter                           | 1 every 2 months   |
| Web Presence                         | News pieces on website               | 1/week<br>250 of visitors<br>400 page views  |
| Digital community interaction        | Twitter /Facebook                    | min. 3 Tweets/week<br>Multiple Tweets for promotional campaigns and events.<br>KPI: increase female followers from 26% to 35%.<br>Flash report monitoring on core statistics                                     |
|                                      | LinkedIn                             | Min. 1 post/week with blogs on training and other events.<br>Flash report monitoring on core statistics.   |
|                                      | YouTube                              | Min. 1 project video/year for newcomers.<br>Min. 3 training promotional videos.<br>min 2 posts/month on the online training material (FB, Twitter)<br>Flash report monitoring on core statistics                 |
| Physical events and local activities | Conference                           | 50 attendees per conference<br>All stakeholder groups<br>Number of testimonials (clustered into young people, women, academies and research, industry)   |
|                                      | Webinar                              | Min 1 every 3 months<br>6 webinars in the entire project period (M1-36)  |
| Non-Scientific publications          | Portal Magazine or other publication | 1 News piece content tailored to MaX   |



### 3. MaX results and assets for dissemination & communication

In the following strategy set out, the dissemination, communication, and engagement efforts will follow a clear process which can be synthesised as follows:

- Identification of a tangible project results;
- Definition of their availability date;
- Agreement between the partners of the dissemination and communication assets on the basis of which to develop the stakeholder engagement activities.

In view of dissemination, communication, and engagement efforts, the expected MaX results can be summarized as follows:

- MaX flagship codes
- MaX products
- MaX with integrated services
- MaX with Materials Cloud platform
- MaX Exascale
- MaX training and training material

#### 3.1 MaX Flagship Codes

MaX is a catalyst to maintain and enhance Europe's leadership: a pan-European central hub for developers and users of materials simulations. European codes will be strategically positioned to face the challenges of the pre-exascale and future exascale infrastructures due to the activities designed within the CoE, and the MaX flagship codes will be ready for deployment in pre-exascale machines at the end of the project, and prepared to adapt to the as of yet unknown architectures of the future exascale machines, owing to the work in modularisation and advanced programming models, and the continuous co-design activities that will adapt to upcoming architectures. Aligned with the current efforts of Europe not to be "deprived of strategic know-how" in HPC infrastructure, MaX ensures that it keeps the knowhow and federates the ecosystem in the materials science domain, critical for the competitiveness of any advanced society.

**Table 5: MaX Flagship Codes**

| Name             | Code Description   | License | Main Developers within MaX | Contact Person  |
|------------------|--|---------|----------------------------|-----------------|
| QUANTUM ESPRESSO | the prime open-source (set of) code(s) for quantum materials modelling using the planewave pseudopotential method. | GNU-GPL | SISSA, CNR, CINECA         | Paolo Giannozzi |



|        |  |         |         |                    |
|--------|--|---------|---------|--------------------|
| SIESTA | a density-functional code able to perform efficient electronic structure calculations and ab initio molecular dynamics simulations of molecules and solids.  | GNU-GPL | ICN2    | Pablo Ordejon      |
| YAMBO  | a code that implements ground-state as well as excited-state properties in an ab initio context.   | GNU-GPL | CNR     | Andrea Marini      |
| FLEUR  | a code family for calculating ground state as well as excited-state properties of solids within the context of density functional theory. A key difference with respect to the other MaX-codes and indeed most other DFT codes lies in the treatment of all electrons on the same footing.   | MIT     | JUELICH | Stefan Blügel      |
| CP2K   | 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 | CSCS    | Joost VandeVondele |
| BIGDFT | an electronic structure pseudopotential code that employs Daubechies wavelets as a computational basis, designed for usage on massively parallel architectures.  | GNU-GPL | CEA     | Luigi Genovese     |
| AiiDA  | a Python materials' informatics framework to manage, store, share, and disseminate the workload of high-throughput computational efforts, while providing an ecosystem for materials simulations where codes are automatically optimised on the relevant hardware platforms, and complex scientific workflows involving different codes and datasets can be seamlessly implemented and shared. | MIT     | EPFL    | Nicola Marzari     |

### 3.2 MaX Products

The following additional **MaX products** will be available in the MaX website where all the information is readily accessible and reusable by the research market, developers, end users and the general public in adopting the current codes to the commercial services. (See Figure 8: MaX branding logo for products and services).



#### Product list:

- Software applications/releases
- Libraries
- Algorithms
- Tools
- Protocols
- Publications

### 3.3 MaX Services

MaX has developed **services and technical support** that MaX is offering to the general public will be showcased and available in the MaX website, including:

- Quantum as a Service
- Basic support
- Advanced support
- Service helpdesk

(See Figure 8: MaX branding logo for products and services).

### 3.4 Materials Cloud Platform

Materials Cloud is an open science platform designed to enable seamless sharing and dissemination of resources in computational materials science. These include educational material, interactive tools, simulation services, curated and raw data. As such, Materials Cloud will be a primary instrument for the dissemination of MaX results to the broad community of users.

Materials Cloud is powered by AiiDA, a python framework for managing and tracking materials science calculations. Thanks to AiiDA, Materials Cloud provides access to the full provenance of materials science calculations, that is, not only the final results of such calculations, but to every step along the way. More information on the development of the platform is reported in D5.1.

To broaden the use of Materials Cloud, MaX has launched a communication and dissemination strategy focused to the HPC community. This involves a series of presentations to conferences and organization of seminars and tutorials.

A number of training events are planned as described in D8.1 “Training and Education Programme”. In addition, a series of courses are planned to introduce AiiDA and the Materials Cloud platform to PhD students, such as the PhD Course on high-throughput simulations and web platform deployment (with introduction to AiiDA and Materials Cloud), given by Giovanni Pizzi at University of Udine (Italy), from May 7 to May 10, 2019.

Importantly, tutorials make use of the Quantum Mobile, a virtual machine that comes with a collection of quantum simulation codes (Quantum ESPRESSO, Yambo, Fleur,



Siesta, Cp2k), which are set up and ready to be used through AiiDA. New releases of Quantum Mobile will be implemented to keep it up to date with the codes. Moreover, it is planned to integrate the Materials Cloud Archive in B2FIND to make it findable and accessible to all the EOSC-Hub community.

In order to reach both the HPC community and the general public, Materials Cloud and AiiDA activities are advertised using the AiiDA mailing list, with periodical tweets using the @aiidateam Twitter profile and with the publication of posts on the AiiDA Facebook page.

### 3.5 Exascale

MaX is focusing on scaling up a set of widely used materials science codes (MaX flagship codes, refer to table 5), towards upcoming exascale architectures, and to codesign activities that rely on close collaborations with hardware industry stakeholders as well as other components of the EuroHPC Ecosystem. The main objectives are detailed in D4.1.

MaX will continue the close interaction with the relevant communities through one-to-one meetings and a series of talks and presentations. Examples include the presentation by Carlo Cavazzoni in the Codesign session of the EuroHPC Summit Week (May 13-17) in Poznan, Poland, as well as the presentation “HPC, HTC and HPDA convergence in the MaX CoE” given by Sebastiaan Huber (EPFL) in the same event.

### 3.6 Training and training materials

MAX will organize training events structured as workshops, courses, tutorials, schools and hackathons with the purpose of reaching a wide community, both in academia and industry. To this aim, MAX CoE will coordinate most of these training activities in collaboration with CECAM, Psi-k and ICTP. This will allow us to benefit from their established tradition and user base in the education domain, thus contributing to the engagement of different communities. The training will be dedicated to both developers and academic and industrial users. A list of the events already completed and planned can be found in the Training & Education Programme, D8.1. In addition, MAX will also contribute to coordinate initiatives, which will be organized with PRACE and the FocusCoE or in collaboration with other CoEs. In order to maximize the attendance of all the events and attract interest from the HPC community and potential users of the MAX flagship codes, such activities will be publicized in the MAX website, advertised and covered *via* the MAX communication channels (Twitter and LinkedIn accounts) and promoted through news and mailing lists. In addition to the impact on training, some of these events (e.g. hackathons) offer a great opportunity for disseminating MAX products, as e.g. the libraries produced in WP1.



The material produced for all training activities, e.g. hands-on schools on MAX flagship codes, will be made publicly available in MAX dedicated channels interlinked with the main MAX website. This includes tutorial texts and recorded video lectures. Video lectures as well as promotional training videos will be also uploaded in the MAX youtube channel.

#### 4. Communication and Dissemination Plan

To support its goals and generate impact, MaX implements a 36-month communication strategy aimed at supporting the dissemination and stakeholder engagement goals and targets of the project, coordinated under WP9 – Communication and Dissemination Strategy & Stakeholder Engagement Plan, drawing on the extensive know-how, experience, and network within and of the MaX consortium.

Throughout the duration of the project, all MaX partners contribute to community development and stakeholder engagement on a continuous basis as part of the project's communication plan. Having an effective communication plan is key to paving the way to dissemination and exploitation of results, to which all partners have committed according to availability dates and beyond the project lifecycle.

Assets to support these goals include an already strong community of all EU HPC Centres, and the wide users communities of the flagship codes. The involvement of many MaX teams in European organisations focused on materials and simulations, like CECAM, Psi-k and the EMMC, will be instrumental in the engagement and participation of the community at large, by their involvement in scientific, training and outreach activities, including specialized workshops and hackathon events.

Moreover, MaX benefits from leverage coordination with other CoEs and the Focus CoE project, and collaboration with established organizations that can support the engagement of communities, such as EOSC in general and EOSC-Hub. The various stakeholder groups defined in Table 1 will be targeted by a number of engagement activities and campaigns aimed to enable 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.

##### 4.1 MaX Community

MaX community builds on developers of the leading EU open source community codes in the materials domain, five leading European HPC centres, two technology partners, and training and communication experts. Since the start of the project the community has been expanding already thanks to social media activity, engagement during events and partner and linked third parties reachout.



At the time of writing, MaX is expanding its community through LinkedIn (139 connections at the time of writing) and Twitter (634 followers at the time of writing), resulting in a total of 736 community involved. Overall acquired contacts are spanning across all the stakeholder profiles of Table 1. A high number of profiles acts as a multiplier and as an influencer generating an elevated resonance among our stakeholders. Our social media communication will leverage on their network of followers to increase the project's visibility.

Annex III lists some of the channels that are following MaX's Twitter account at the time of submission the deliverable (May 2019), representing relevant numbers in terms of followers in fields that are of interest to MaX's community. Continuous community monitoring is performed by Trust-IT and it will be circulated regularly to all Consortium Partners.

#### 4.2 Content Driven approach

The communication and dissemination plan will concentrate its efforts around copywriting and producing engaging, stimulating and impactful content. Our editorial planning will include the regular publication of articles covering partners' highlights, MaX in practice stories, and a news piece to send to MaX website news board every month.

MaX contents aim to directly fuel user participation to MaX processes, therefore maintaining coordination with all of the more technological WPs one through to five as well as the training and competence centres and the various engagement drivers. The activities carried out will ensure sufficient visibility to sustain the engagement figures and achieve the necessary concertation levels with the related initiatives and the Coordination and Support Action (FocusCoE) funded under the same call.

A set of **6 specific webinars** will be organised and broadcasted (and eventually published for playback) to support the training elements in the other WPs. The implementation and maintenance of all graphic design & branding will also be managed under this task. It will cover the coordination and production of MaX branding and material and visual presentations. This includes all categories of MaX related dissemination material as well as event or milestone specific graphic packages (workshop meeting logos, badges, posters, giveaways) and material targeting specific stakeholder groups. Graphics also include the generation and update of web based templates and revamp of the web graphical layouts of the MaX web platform.

#### Communications mapped to outputs

The purpose of creating the timeline as outlined in Annex 1 Timeline [M1-M12] is to map the results as well as to match the outreach activities as indicated in the Timeline itself. As already highlighted, the main results deriving as a result of such activities will be pulled out and registered in the monthly "Flash Report".



## Examples of the content-driven approach for MaX

The communication strategy developed in WP9 will produce easy-to-read digests of deliverables for stakeholders, communities, partners, and reviewers so that this journey will be continuously communicated and clear for everybody. These digests will show the work that the project is continuously carrying out over the course of its 36-month duration.

Efforts have been made to show the project partners who will, over the next 36-months, be building the new cloud-based infrastructure to make data, tools, and training available for scholars, developers and the general public interested in the High-Performance Computing community in the field of materials design. This includes all categories of MaX related dissemination material as well as event or milestone specific graphic packages (workshop meeting logos, badges, posters, giveaways) and material targeting specific stakeholder groups. Graphics also include the generation and update of web based templates and revamp of the web graphical layouts of the MaX web platform. In addition, content in the revamp web platform will showcase the MaX flagship codes, services and products, and exascale with the relevant testimonials from the experts in the HPC and MaX partners.

Figure 5: Example of MaX written article

### MaX CoE Cooperation on EOSC-hub Week 2019



The Materials design at eXascale (MaX) is one of the High-Performance Computing Centers of Excellence (HPC CoE) that was invited to showcase how MaX is seamlessly integrating with EOSC and how Aida and Materials Cloud tools are paving the way ...

### EuroMPI 2019: Call for Papers



ETH, Zurich, Switzerland, September 10-13, 2019. The EuroMPI conference is since 1994 the preeminent meeting for users, developers and researchers to interact and discuss new developments and applications of message-passing parallel computing, in particular in and related to the Message ...

### 5 Reasons Why You Should Apply for Summer School on Advanced Materials and Molecular Modelling with QUANTUM ESPRESSO



The QUANTUM ESPRESSO Foundation and the EU MaX Centre of Excellence for Supercomputing Applications, in association with the Jožef Stefan Institute, are holding a "Summer School on Advanced Materials and Molecular Modelling with QUANTUM ESPRESSO" this coming 16-20 of September ...

### CECAM Summer School on Classical Molecular Dynamics for Material Science, Nanotechnology and Biophysics @ SISSA

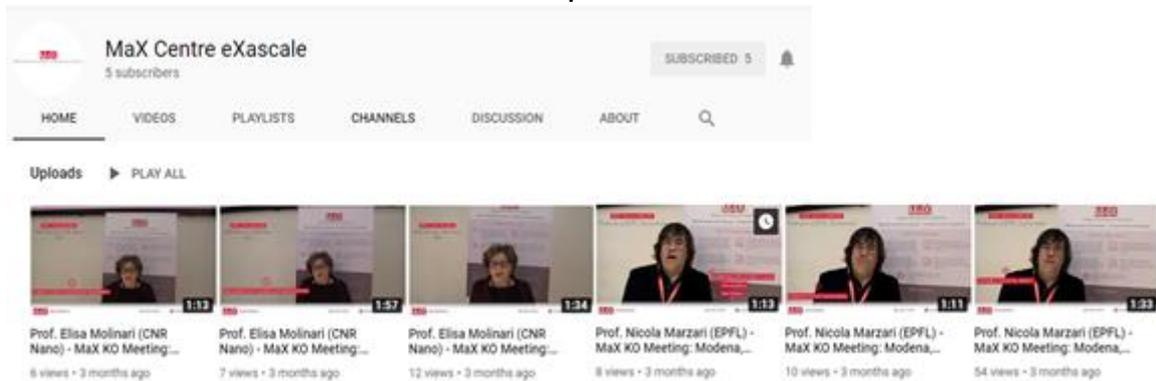


June 10 – June 21 2019, Sissa-Trieste | Italy The School is primarily intended for undergraduate students in Physics or Chemistry who wish to become familiar with up-to-date Molecular Dynamics simulation techniques. Due to recent technical problems on the Cecam ...



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**Figure 6: Example of MaX videos from the Kick-Off Meeting event providing the testimonial from the MaX partners**



WP9 team work hand in hand with WP8 Training & Uptake, leveraging on state-of-the-art communication activities to effectively engage with the MaX stakeholders. Every addition or update on the training initiatives and training and education program will be highlighted and promptly communicated.

MaX’s content will be made available under the conditions of a Creative Commons open license, in line with the European Commission’s approach towards research data which is “as open as possible, as closed as needed”. The preferred license for the project’s communication output is a Creative Commons Attribution 4.0 International License.

### 4.3 Visual identity and branding

A consistent visual identity will be used for all communication and dissemination activities. Templates for external communication and documents will be provided. Presentations templates are already available including on the last page a call to join the MaX community and to connect with our main channels.

**Figure 7: Presentation Template last page with call to action to join the MaX community**





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There will be a final branding alignment across all formats and channels used to reach stakeholders, spanning the training, MaX flagship codes, products and services, and integrated news, social media, brochures, banners, posters, and other collaterals.

Figure 8: MaX branding logo for products and services



Figure 9: MaX dedicated branding section for the flagship codes



#### 4.4 Liaison with Training

This section is to highlight the partnership with WP8, led by Daniele Varsano (CNR), with the purpose to achieve the common goal to remove the barriers that prevent MaX 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.

In liaison with WP8, different actions will be planned to train new generations of developers and code users. Within each action, special attention will be devoted to young people and women in research and technology.





## 4.6 Dissemination outreach

### 4.6.1. Industrial Engagement

Broader engagement of industry is a key target of the MaX CoE as a whole. **All MaX activities** will especially address industrial users. In addition, the dissemination plan encompasses the following **dedicated actions**:

- MaX supports the forthcoming National Competence Centres to be developed in the EuroHPC framework: these Centres will especially emphasize industry- and SME-related activities. MaX will organize a special effort to provide material, consulting and support to these hubs which can be important for a widespread interface with industry. In addition, MaX will contribute to SME projects and applications to EU programmes, especially the planned EuroHPC action "Stimulating the innovation potential of SMEs";
- Dissemination activities towards selected industrial sectors: this will be the core of the FocusCoE CSA, which plans to coordinate the participation of several relevant CoEs in fairs and other sectoral events in order to strengthen the impact of each CoE. MaX will collaborate with FocusCoE to make these activities the most effective and promote MaX codes and products;
- Engagement of independent software vendors (ISVs) in MaX events (including training and hackathons), as well as face to face meetings: this activity is not only relevant in view of specific agreements with the ISVs companies, but also as a vehicle towards end-user companies. We have experienced that ISVs offer user-friendly access to some MaX flagship codes with very broad impact especially in industrial environments including SMEs;
- Engagement of Hardware (HW) companies: these are interested in the codesign process and in boosting the adoption of their technology: a close interaction is planned under the coordination of WP4 and in collaboration with all HPC Centres.

In addition, WP9 has generated a database to collect success cases obtained in the first phase of MaX, in order to showcase the relevant result related to industry. The file will be used to finalize the content for the suggested webinars which will focus on the industry market. And, also to generate the relevant news piece aiming to reach the industry experts and early researchers, HPC end users as well as the general public.

The following questions have been identified and shared among the MaX consortium:

- Q1. Which MaX services can be oriented to industry?
- Q2. Identify which industry you have engaged with and with what results?
- Q3. How do the MaX products and/or services support (or have supported) this industrial partner?
- Q4. What need are you trying to address for them?
- Q5. What dissemination strategy is being used/or will be used to promote MaX results?

Stronger ties are being established with the EMMC (European Materials Modelling Council) to establish a direct liaison and relationship, besides the existing collaborations with individual MaX partners (EPFL and ICN2), in order for the MaX community to attain



a stronger Industrial engagement. Plans for the future include (i) attending the industry workshop taking place in Turin (08/10 July 2019) to showcase MaX findings and codes among a targeted audience that includes such as PostDocs, Academic research, Industrial R&D group leaders or advanced PhD students who actively work on materials modelling software and codes; (ii) organising a co-located event in the process of collecting some specific use cases where industry is particularly relevant with EMMC support, and an industry-focused Webinar to showcase 2 success stories as well as some EMMC (or other industry) spokesperson to present the Industrial Materials Modelling Simulation landscape in Europe. EMMC also carries out relevant training workshops (supported also by WP8) on Business Models for material modelling software. The consortium will consider weaving some of the training workshops or the webinar activities MaX organises.

#### 4.6.2. Public Engagement

- The MaX team generated a complete visual identity rehaul of the new MaX website focusing on the user experience with a more user friendly, easy to access and dynamic appeal to the MaX community as well as potentially to a general public. The idea is also showcasing the results of the previous MaX phase, products and services that are publicly available.
- Workshops, as well as training events organized by WP8, will be opportunities to share MaX findings with new generations of developers and code users.
- MaX team is planning to join other public events such as European Research and Innovation Day, the ESOF2020 event and Researcher's Nights. Within each action, special attention will be devoted to young people and women in research and technology.
- The consortium has scheduled to carry out a video to explain MaX in a nutshell and what kind of impact could be suitable for a general public audience. The video will complement the interview videos that are already available on YouTube and the websites for viewing.

Finally, from a civil society perspective, MaX will try to fill a recognised gap through its engagement and synergies with Missions Publiques (<https://missionspubliques.org/en/>), to leverage its ongoing Stakeholders strategy to involve the general public: Mission Publiques aims to bring citizens into policy that interacts directly with citizens on society. MaX will also engage with the International Civil Society Centre <https://icscentre.org/> as well as international charities working towards their digitisation programmes.

#### 4.6.3. Pan-European Dimension

MaX consortium will put into place profitable/synergistic interactions with other CoEs



and European projects, e.g. the EU Graphene Flagship project. Here are some engagement initiatives:

- A MaX-Graphene Flagship (GF) joint event will be held in Helsinki Finland during the Graphene Week (23-27 September), bringing together the latest innovations and leading-edge technology and research on graphene, with experts related to industry and academia. A joint MaX-GF scientific workshop on “High performance computing for 2D materials research” is planned, together with a joint policy session on “European HPC initiatives and 2D materials research: collaborating and funding opportunities”.
- The interactions of MaX with the Competence Centres that are planned by EuroHPC will be relevant to promote collaborations in countries which are not yet directly involved in MaX activities. As mentioned in section 4.6.1., MaX will organize a special effort to provide material, consulting and support to these hubs, and pay constant attention to its pan-European impact;
- In addition, to promote pan-European collaborations and coordination MaX plans to organize events in countries that are not yet leading in the materials research domain or HPC. Scientific organizers from those countries will be involved as much as possible. Three perfect examples are: (i) the Summer School on Quantum ESPRESSO that will be organized by MaX in Slovenia in September 2019, jointly with the Jozef Stefan Institute (Ljubljana), Ruder Boskovic Institute (Zagabria) and the Institute of Physics (Belgrade); (ii) the School on First Principles Simulation of Materials with SIESTA, organized by MaX in Belgrade in November 2019, in collaboration with the University of Belgrade; (iii) the Aiida tutorial, that will be organized by MaX in Vilnius, Lithuania, in Spring-Autumn 2020, jointly with the Vilnius University. For additional details see D8.1.

#### 4.7 Example of messaging and value proposition

In line with current trends, MaX’s social media activities are focused on **actionable, goal-oriented, highly visual, content-rich** posts that combine insightful, yet concise text content, hashtags, engaging images and videos. For example, the short post below (Figure 11) focuses on the MaX cooperation on the EOSC Hub Week 2019 presenting the “Pathways for EOSC-hub and MaX collaboration” which opens the opportunity to explore the collaboration between EOSC and HPC CoEs and sought to understand the synergies and complementarities on which both EOSC-Hub and the HPC CoEs can capitalise on for mutual benefit to how EOSC-hub can further support HPC CoEs activities.



Figure 11: Tweet on MaX cooperation on the EOSC Hub Week 2019



The activities on the various social media channels will also be supported by newspaper pieces, such as the first news piece of the MaX participation to the EOSC Hub Week 2019 and the impact of the participation of MaX on the event. While the simple posts with text and visuals are meant to have an immediate impact in terms of creating interest, press releases deliver relevant results also for targeting the specialised journalists and other multipliers. The fact of publishing the press release on social media platforms such as LinkedIn, populated by a lot of potential stakeholders, is a great advantage as it allows interested readers to find out more by even just having a short look at the article.

An effective event campaign offers the chance to underline the attributes of MaX to anyone who gains interest by reading about it in the shorter posts, and it also involves important SEO benefits, thereby increasing traffic to the website (see Figure 12 below).

Figure 12: Pre-event News piece on Pathways for EOSC-Hub and MaX collaboration

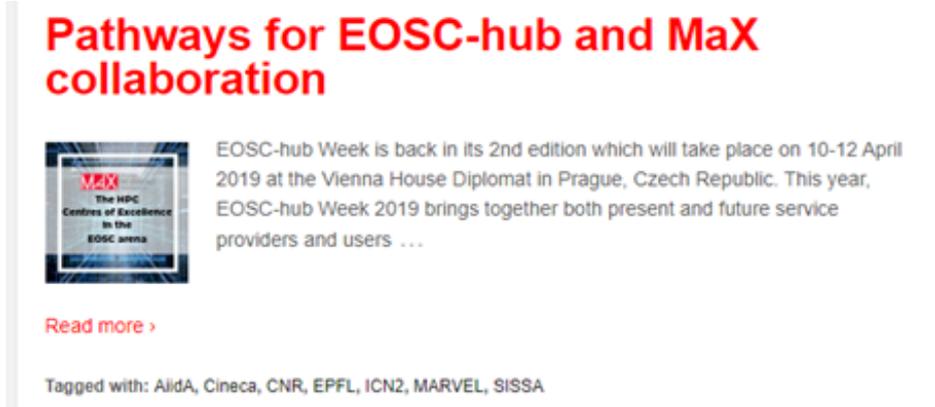


Figure 13: Post event News pieces on MaX cooperation on the EOSC Hub Week 2019

## MaX CoE Cooperation on EOSC-hub Week 2019



The Materials design at eXascale (MaX) is one of the High-Performance Computing Centers of Excellence (HPC CoE) that was invited to showcase how MaX is seamlessly integrating with EOSC and how Ailda and Materials Cloud tools are paving the way ...

[Read more >](#)

Tagged with: CNR, EPFL, ICN2, SISSA

### 4.8 Visibility at Events planning

Every MaX related event, workshop, or webinar will be communicated and posted on the dedicated section of MaX's website and social media channels, covering pre-, during-, and post-event activities.

Collaterals will help in building the MaX identity and implementing the Dissemination & Outreach strategy. Branded MaX notebooks and pens and a MaX official banner are already available and will be brought and exposed at MaX related events (examples see figure 14).

Figure 14: Example of MaX Collaterals



MaX related events will be promoted through social media activities and through dedicated campaigns. Prior to the event, we will promote "save the date" posts, publish



the event and the agenda on MaX’s website, track all links involved in the campaign, formulate dedicated hashtags and create articles, videos and banners. These events will receive an appropriate follow-up through PPT publication, wrap-up posts, and video interviews from the event, giving a balanced and fair visibility to each partner. All MaX events that are directly related to MaX as well as those that represent a promotion opportunity for the consortium will be listed in a dedicated event database, shared with all partners and linked third parties. The current event file shows the type of event, the related task, leading participant, communities addressed and the approximate number of participants to be reached, as well as the relevance, place, dates, links and further information (for a compromised version see Annex IV).

### 5. Monitoring the Impact

WP9 will set up a Monitoring Service tailored to MaX needs to measure the impact achieved by the carried out communication activities. We will set up a shared dashboard, that will visually render all the data from our communications and online activities for a continuous and easy monitoring of KPIs. Necessary adjustments will be made during the course of the project. Alerts about the MaX community will be activated to keep track of the fuss around the project.

KPIs tracker information tool is displayed in the figure below (Figure 15):

Figure 15: MaX KPI Tracker

|   | Toolkit element  | KPIs and Qualitative Metrics  | KPI (total numbers over 36 months)   | Category (UC - Uncontrollable, C - Controllable) | Target (based on GA)  | Running Score | Dec 2018 | Jan 2019 | Feb 2019 | Mar 2019 | Apr 2019 | May 2019 |
|---|--|---|--|--|---|---------------|----------|----------|----------|----------|----------|----------|
| KPI 9.1   |  | KPI 9.1   | Total number of invited talks to conferences and schools plus total number of publications   | UC   | 13 Community Events + 13 Written Article by M12                                   | 14            | 0        | 2        | 2        | 3        | 4        | 3        |
| KPI 9.2   |  | KPI 9.2   | Total number of people in the MAX network (social media, registered to the newsletter, event participants)   | C  | 1000 MaX Networks by M12 (internal target)<br>(average of 34 new followers/month) | 763           | 12       | 57       | 18       | 28       | 36       | 27       |
| Communication strategy: awareness-raising and continuous stakeholder engagement | Search Engine Optimization-driven website revamp tailored to MAX; content-rich approach for this project entry point | Regular content creation by copywriters and partner contributions.  | Weekly updates. Min. 1 content piece. Flash report monitoring on core statistics (e.g. number of visitors, page views etc)   | C  | 57 News Piece by M12<br>(1 news piece/week)                                       | 22            | 0        | 2        | 7        | 3        | 8        | 2        |
|   | Community building through social media: Twitter and Facebook  | Build on current results; increase followers and interactions especially with young people and women.           | min. 3 Tweets/week. Multiple Tweets for promotional campaigns and events. KPI: increase female followers from 26 % to 35 %. Flash report monitoring on core statistics | C  | 171 Tweets by M12<br>(3 tweets/week)  | 115           | 13       | 24       | 18       | 24       | 21       | 15       |
|   | Community building through professional networks: LinkedIn   | Setup LinkedIn page. Active participation in LinkedIn Groups (see table below). Updated profile every 6 months. | Min. 1 post/week with blogs on training and other events. Flash report monitoring on core statistics.  | C  | 57 LinkedIn Post by M12<br>(1 linkedin post/week)                                 | 39            | 0        | 9        | 9        | 9        | 10       | 2        |



## 6. Conclusions

The present document is the cornerstone for all Dissemination and Outreach activities to be carried out in MaX over the project's lifetime. The main conclusions are:

- The “MaX Communication & Dissemination Strategy & Stakeholder Engagement Plan” is tightly linked to the project results and therefore is to be considered as a living document: it will be up to the “Engagement, Communication, Dissemination & Uptake” work package to timely update it whenever necessary.
- WP9 activities in the first three months of the project have been conducted with good coordination and produced tangible results, including completion of project branding, launch of the new website, visibility at events and production of a wide number of collateral.
- A first timeline for the initial period has been developed and it will be followed as part of WP9 as well as an overview from M6-M36 for MaX.
- All Consortium partners have shown good and continued alignment and high commitment in the development and implementation of the present plan.

As a summary, in the first months of the project, and as outlined in this document, we are making sure that there is a plan to address all prospective stakeholders. A strategy that builds on thematic services experience, competence center development as outlined in the grant agreement, and business pilot showcasing is designed. The communication and key events are identified as well. In this respect when a prospective stakeholder wishes to engage with MaX, we will have in place the tools to support the engagement and induction process to engage not only the technical stakeholders but industry as well as the general public.

## 7. References

MaX Grant Agreement

<https://cordis.europa.eu/project/rcn/220063/factsheet/en>

EOSC Hub Communication and Stakeholder Engagement Plan

<https://www.eosc-hub.eu/sites/default/files/EOSC-hub-D3.1.pdf>

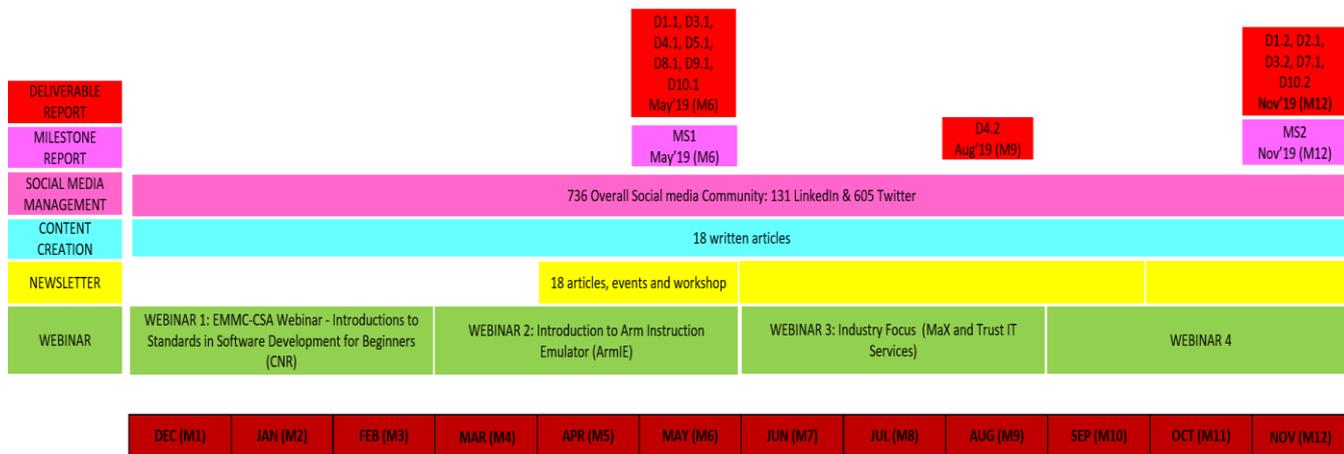


Deliverable D9.1  
MaX Communication and Dissemination Strategy & Stakeholder Engagement Plan

Annex I - Timelines M1-12



TIMELINE OF REPORTS AND DELIVERABLE



TIMELINE OF EVENTS AND WORKSHOPS



Legend: MaX Stakeholders

- EU and members states institutions
- EU HPC ecosystem (HPC centers, Prace, Eudat)
- Hardware Manufacturers
- Industrial and Academic end-users
- Independent software vendors (ISVs), code developers
- Large scale experimental facilities
- Education system



Annex II - Database Rationale and Image

● Stakeholder Database

An online shared system to keep track of the different stakeholders and the actions taken towards each community group together with the indication on who is responsible for updating which part of the system. The general approach will be that whenever a MaX partner team member is in contact already with the community, he/she will be responsible for the specific engagement with the community; for new communities (not in contact already with any MaX partner) will be assigned to one of the task 9.2 team members in coordination with WP8.

| Type of Stakeholder  | Affiliation/Institution           | Extended Name of the Community                       | Description                        | Disciplinary area                        | Main contact within the entity     | First Name                                    | Surname                                      | Gender                                 | Role  | Owner in the project   | Priority  | Why to engage with them   | Channel to reach them  | Website URL                         |
|--|-----------------------------------|--|------------------------------------|--|------------------------------------|---|--|--|---|--|---|---|--|-------------------------------------|
| stakeholders to allow targeted communication or messages to be created | name of the community/association | Extended name of the community                       | short description of the community | main scientific domain for the community | reference person for the community | FIRST NAME reference person for the community | LAST NAME reference person for the community | gender reference                       | identify the role of the contact within the community | who within MaX team is responsible for the engagement with the community | priority in the engagement which will be decided based on the trust | which is the main reason and objective of the engagement as described by the specific community | best channel to be used to reach the expected engagement as described (email, twitter or linkedin) | Affiliation/institution website URL |
| EU HPC ecosystem (*)   | BioExcel                          | Centre of Excellence Centre of Excel                 | Biomolecular Res                   | Miriam White                             | Miriam                             | White   | Female                                       | Dissemination Or Trust IT Services     | Euro HPC CoE  | To synergise with one m.white@eccp.ed.ac.uk                              | https://bioexcel.eu   |   |  |                                     |
| EU HPC ecosystem (*)   | ChESSE                            | Centre of Excellence Project under B. Exascale       | supercomputing                     | Armau Foich                              | Armau                              | Foich   | Male   | BSC Principal Inv. Trust IT Services   | Euro HPC CoE  | To synergise with one armau.foich@bsc.es                                 | https://www.bsc.es  |   |  |                                     |
| EU HPC ecosystem (*)   | CompBioMed2                       | Computational I, Computational II, Computational III | Emily Lumley                       | Emily                                    | Lumley                             | Female  | Project Coordination Trust IT Services       | Euro HPC CoE                           | To synergise with one e.lumley@ucl.ac.uk              | https://www.compbio.ac.uk  |   |   |  |                                     |
| EU HPC ecosystem (*)   | EoCoE                             | Energy oriented - The Energy orient                  | Energy oriented                    | Edouard Audit                            | Edouard                            | Audit   | Male   | Project Coordination Trust IT Services | Euro HPC CoE  | To synergise with one contact@eocoe.eu                                   | https://www.eocoe.eu  |   |  |                                     |
| EU HPC ecosystem (*)   | EnVIACE                           | Centre of Excellence CoE in Simulation               | Simulation of W. Joachim Biercamp  | Joachim                                  | Biercamp                           | Male  | Project Coordination Trust IT Services       | Euro HPC CoE                           | To synergise with one biercamp@divz.de                | https://www.enviace.eu   |   |   |  |                                     |
| EU HPC ecosystem (*)   | EnVIACE                           | Centre of Excellence CoE in Simulation               | Simulation of W. Chiara Beardsom   | Chiara                                   | Beardsom                           | Female  | Project Officer Trust IT Services            | Euro HPC CoE                           | To synergise with one beardsom@divz.de                | https://www.enviace.eu   |   |   |  |                                     |
| EU HPC ecosystem (*)   | E-CAM                             | European HPC CoE-CAM is an e-Inf                     | An e-Infrastructure                | Ana Catarina Mendonca                    | Ana Catarina                       | Mendonca                                      | Female                                       | Project Coordination Trust IT Services | Euro HPC CoE  | To synergise with one ana.mendonca@epf.c                                 | https://www.e-cam.eu  |   |  |                                     |
| EU HPC ecosystem (*)   | EXCELLERAT                        | The European CoE EXCELLERAT is b                     | Engineering App                    | Bartholomäus Koller                      | Bartholomäus                       | Koller  | Male   | Contact person in Trust IT Services    | Euro HPC CoE  | To synergise with one buehler@hirs.de                                    | https://www.excellerat.eu   |   |  |                                     |
| EU HPC ecosystem (*)   | HIREAC - HIDALGO                  | HPC and Big Data HIDALGO bridges                     | HPC and Big Data                   | Madeleine Gray                           | Madeleine                          | Gray  | Female                                       | Communication Trust IT Services        | Euro HPC CoE  | To synergise with one madeleine.gray@bsc.a                               | https://www.hireac.eu   |   |  |                                     |
| EU HPC ecosystem (*)   | PDP                               | Performance Opt The EU H2020 P                       | Performance Opt                    | Yara Duvenger                            | Yara                               | Duvenger                                      | Female                                       | PDP Project manager Trust IT Services  | Euro HPC CoE  | To synergise with one yara.duvenger@bsc.a                                | https://pdp-coe.eu  |   |  |                                     |

● MaX Services, Results & Assets and Flagship Code\_3 Questions

An online shared system to consolidate all the MaX Services, Results & Assets and the 3 questionnaires to each WP leader to generate the detailed information about each MaX flagship code based on the first phase of the project.

● MaX Flagship Code\_3 Questions

| Code            | Responsible          | Co-Responsible       | Co-Responsible    | Responsible             | Code | Code   | Code   |   |
|-----------------|----------------------|----------------------|-------------------|-------------------------|------|--|--|---|
| CPXK            | Jozsef Vandyvondiele | kozhenyikv@cs.cu.ch  | Anton Kozhenyikov | kozhenyikv@cs.cu.ch     | CSCE | CPXK code is well known in the materials science and quantum chemistry communities. Its rich functionality and a long list of features make it a "go-to" atomic simulation and a useful tool for many researchers. In the context of MaX-2 project CPXK code will be optimized for emerging HPC architectures and extended with the innovative capabilities. In particular, we enable enhanced GPU performance for key aspects of the code, that are important for the simulation of large systems, or beyond DFT (DFT, etc). There is a large user base in Switzerland that relies on these capabilities. Furthermore, pre-exascale architectures such as Summit (NV based) are being targeted, with user bases overseas. | Each researcher measures the code quality differently and there is no standard metrics to tell which code is better. CPXK can do a lot of things efficiently, other things it can't do. It really depends on the problem and the choice of methods to solve it. In the particular case of this development, we aim for enabling Monte Carlo and molecular dynamics capabilities on top of DFT. These are unique strengths. In terms of code development practice CPXK team follows very high standards for source code organization, verification, validation and the release cycles.  | We believe that any open source contribution to the scientific software development is beneficial for the society in the long term. Furthermore, this focused effort on accelerated computing, is fully in line with known exascale plans, and will benefit the materials community as a whole, keeping at the edge of supercomputing.  |
| AiDA            | Nicola Marzi         | nicola.marzi@epfl.ch | Spyros Zoupanos   | spyros.zoupanos@epfl.ch | EPFL | AiDA is a tool (a) to perform hundreds of thousands of simulations without the need to monitor them closely, (b) to store the results efficiently to a database, the file-system or a storage service, (c) to keep track of their simulations via the automatically generated provenance graph, (d) to analyse research results by querying the provenance graph via a powerful query tool directly in a high-level programming language like Python, (e) to automate the scientific work with workflows and (f) to share results.   | AiDA is a scalable simulation platform with efficient provenance support and workflows. It doesn't just facilitate the execution of high throughput calculations but enables the analysis of results using a powerful querying tool, the sharing of the results among users and is compatible with a large number of physics simulation codes. All these advantages make it unique in the computational science domain.  | AiDA plays a key role to the acceleration of the design and discovery of materials displaying novel physics or improved properties, via high-throughput simulations. Novel materials have applications in various domains of the industry affecting directly or indirectly our everyday life. An example of such application is the improvement of performance of lithium batteries found in numerous devices, or the discovery of new porous materials that can efficiently store methane.   |
| Materials Cloud | Ella Pasaro          | ella.pasaro@epfl.ch  |                   |                         | EPFL | Materials Cloud [www.materialscloud.org] is a web platform developed to help computational materials scientists share their work and promote open science. The five sections of the Materials Cloud platform - LEARN, WORK, DISCOVER, EXPLORE and ARCHIVE - allow the seamless sharing and dissemination of resources such as learning material, interactive tools, curated and raw data as well as the actual calculations underlying published results.  | Materials Cloud is powered by AiDA, which allows to manage and track materials science calculations. It allows researchers to share through Materials Cloud not only the results of their calculations but also every step taken to get there, to download individual files or entire databases with the click of a button, and to browse and query calculations using a web browser. By using AiDA to perform calculations and Materials Cloud to share their results, scientists render their research data complete, fully downloadable, easy to browse and ready to reuse, thus complying with the FAIR data principles (to be Findable, Accessible, Interoperable, Reusable). | Through the dissemination of scientific data, learning materials, and simulation tools, Materials Cloud contributes to advance open science and to accelerate the discovery of novel materials, which have a wide variety of applications ranging from electronics to renewable energy as well as from the pharmaceutical industry to communication technologies. Indeed, the LEARN section of Materials Cloud distributes educational materials for students and universities, while the EXPLORE section and the AiDA Lab provide open access to simulation tools. Curated scientific results with interactive visualizations are displayed in the DISCOVER section, such as the datasets of 20 materials or consistent organic frameworks for methane storage applications. |

● MaX KPI Tracker



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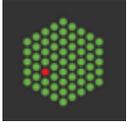
An online shared drive for where we house the internal key performance metrics and score based on MaX grant agreement.

|   | Toolkit element  | KPIs and Qualitative Metrics  | KPI (total numbers over 36 months)   | Category (UC - Uncontrollable, C - Controllable) | Target (based on GA)  | Running Score | Dec 2018 | Jan 2019 | Feb 2019 | Mar 2019 | Apr 2019 | May 2019 |
|---|--|---|--|--|---|---------------|----------|----------|----------|----------|----------|----------|
| KPI 9.1   |  | KPI 9.1   | Total number of invited talks to conferences and schools plus total number of publications   | UC   | 13 Community Events + 13 Written Article by M12                                   | 14            | 0        | 2        | 2        | 3        | 4        | 3        |
| KPI 9.2   |  | KPI 9.2   | Total number of people in the MAX network (social media, registered to the newsletter, event participants)   | C  | 1000 MaX Networks by M12 (internal target)<br>(average of 34 new followers/month) | 763           | 12       | 57       | 18       | 28       | 36       | 27       |
| Communication strategy: awareness-raising and continuous stakeholder engagement | Search Engine Optimization-driven website revamp tailored to MAX; content-rich approach for this project entry point | Regular content creation by copywriters and partner contributions.  | Weekly updates. Min. 1 content piece. Flash report monitoring on core statistics (e.g. number of visitors, page views etc)   | C  | 57 News Piece by M12<br>(1 news piece/week)                                       | 22            | 0        | 2        | 7        | 3        | 8        | 2        |
|   | Community building through social media: Twitter and Facebook  | Build on current results; increase followers and interactions especially with young people and women.           | min. 3 Tweets/week. Multiple Tweets for promotional campaigns and events. KPI: increase female followers from 26 % to 35 %. Flash report monitoring on core statistics | C  | 171 Tweets by M12<br>(3 tweets/week)  | 115           | 13       | 24       | 18       | 24       | 21       | 15       |
|   | Community building through professional networks: LinkedIn   | Setup LinkedIn page. Active participation in LinkedIn Groups (see table below). Updated profile every 6 months. | Min. 1 post/week with blogs on training and other events. Flash report monitoring on core statistics.  | C  | 57 LinkedIn Post by M12<br>(1 linkedin post/week)                                 | 39            | 0        | 9        | 9        | 9        | 10       | 2        |



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Annex III - MaX Twitter followers (April 2019) and possible levers to reach user communities and other stakeholders

| Organization       | Logo  | Twitter Account | Followers | Stakeholder Group                                    |
|--------------------|---|-----------------|-----------|--|
| Horizon 2020       |    | @EU_H2020       | 102.000   | EU and members states institutions                   |
| DASSAULT SYSTÈMES  |    | @Dassault3DS    | 57.500    | Independent software vendors (ISVs), code developers |
| ARM                |    | @Arm            | 57.200    | Hardware Manufacturers                               |
| Utrecht University |  | @UniUtrecht     | 49.000    | Education system                                     |
| TechNative Wire    |  | @TechNativeWire | 38.800    | Hardware Manufacturers                               |
| EMBL-EBI           |  | @emlebi         | 38.600    | Large scale experimental facilities                  |
| Ghent University   |  | @ugent          | 36.800    | Education system                                     |
| EPFL               |  | @EPFL_en        | 33.900    | Education system                                     |
| ETH Zurich         |  | @ETH_en         | 33.000    | Education system                                     |



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|                          |   |                  |        |  |
|--------------------------|---|------------------|--------|--|
| Cray Inc.                |    | @cray_inc        | 13.400 | Hardware Manufacturers                               |
| SUPERMICRO               |    | @Supermicro_SMCI | 10.600 | Hardware Manufacturers                               |
| Ufficio Stampa Cnr       |    | @StampaCnr       | 6.843  | EU HPC ecosystem                                     |
| BSC-CNS                  |    | @BSC_CNS         | 6.696  | EU HPC ecosystem                                     |
| Forschungszentrum Jülich |   | @fz_juelich      | 5.388  | Education system                                     |
| SISSA                    |  | @Sissaschool     | 5.021  | Education system                                     |
| Cineca                   |  | @Cineca1969      | 3.925  | Independent software vendors (ISVs), code developers |
| EUDAT                    |  | @Eudat_eu        | 3.461  | EU HPC ecosystem                                     |
| PRACE                    |  | @PRACE_RI        | 2.943  | EU HPC ecosystem                                     |
| Bright Computing         |  | @BrightComputing | 2.451  | Hardware Manufacturers                               |
| BioExcel                 |  | @BioExcelCoE     | 1.534  | EU HPC ecosystem                                     |

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Stakeholder Engagement Plan

|                       |   |                  |       |  |
|-----------------------|---|------------------|-------|--|
| EOSC Hub              |    | @EOSC_eu         | 1.463 | EU HPC ecosystem                                     |
| ARKA Softwares        |    | @softwaresarka   | 1.360 | Independent software vendors (ISVs), code developers |
| ETP4HPC               |    | @Etp4H           | 1.307 | EU HPC ecosystem                                     |
| CSCS                  |    | @cscsch          | 1.195 | EU and members states institutions                   |
| QUANTUM ESPRESSO      |   | @QuantumESPRESSO | 729   | Independent software vendors (ISVs), code developers |
| NoMaD                 |  | @NoMaDCoE        | 613   | EU HPC ecosystem                                     |
| POP                   |  | @POP_HPC         | 577   | EU HPC ecosystem                                     |
| FZ Jülich-JSC         |  | @fzj_jsc         | 569   | Industrial and Academic end-users                    |
| ClusterVision         |  | @clustervhpc     | 530   | Hardware Manufacturers                               |
| Leibniz-Rechenzentrum |  | @LRZ_DE          | 524   | Industrial and Academic end-users                    |
| CompBioMed            |  | @bio_comp        | 388   | EU HPC ecosystem                                     |



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|            |   |                 |     |  |
|------------|---|-----------------|-----|--|
| CoeGSS     |    | @CoeGSS         | 322 | EU HPC ecosystem                                     |
| E-CAM      |    | @ECAM2020       | 251 | EU HPC ecosystem                                     |
| EsiWACE    |    | @esiwace        | 245 | EU HPC ecosystem                                     |
| AiiDA      |    | @aiidateam      | 230 | Independent software vendors (ISVs), code developers |
| ChEESE     |   | @Cheese_CoE     | 111 | EU HPC ecosystem                                     |
| EXCELLERAT |  | @EXCELLERAT_CoE | 92  | EU HPC ecosystem                                     |
| FOCUS COE  |  | @FocusCoE       | 90  | EU HPC ecosystem                                     |



### Annex IV - Example of events list: December 2018 - September 2019

(MaX-E: MaX event, MaX-T: MaX Training, MaX-C: community/EuroHPC event with MaX participation). The complete list is available in the MaX repository file where you can find the main takeaways of each event.

Repository link:

[https://docs.google.com/spreadsheets/d/14cf311Ph1Z0a4P5CFQB\\_OqcGLRang4raRDMr0WXKA4U/edit#gid=0](https://docs.google.com/spreadsheets/d/14cf311Ph1Z0a4P5CFQB_OqcGLRang4raRDMr0WXKA4U/edit#gid=0)

| Event Name  | Type and Date        | Where            | Participants  |
|---|----------------------|------------------|---|
| MaX Kick-off meeting  | MaX-E 13-14 Dec 2018 | Modena (IT)      | All MaX members   |
| QE developers meeting   | MaX-T 7-8 Jan 2019   | Trieste (IT)     | Paolo Giannozzi, Pietro Bonfà   |
| Novel Materials to rethink the world @ Uniud  | MaX-C 8 Jan 2019     | Udine (IT)       | Nicola Marzari  |
| 19th International Workshop on Computational Physics and Material Science: Total Energy and Force Methods | MaX-C 9-11 Jan 2019  | Trieste (IT)     | Stefano Baroni, Stefano De Gironcoli, Paolo Giannozzi, Andrea Ferretti, Daniele Varsano, Claudia Cardoso, Pablo Ordejon, Nicola Marzari |
| Yambo and QE developers meeting   | MaX-T 14 Jan 2019    | Casalecchio (IT) | Code developers   |
| BIG MAP consortium workshop   | MaX-C 18 Jan 2019    | Copenhagen (DK)  | Elisa Molinari  |
| INTERSECT Kick-off meeting  | MaX-C 5 Feb 2019     | Modena (IT)      | Elisa Molinari, Andrea Ferretti   |
| PRACE 15th Advanced School on Parallel Computing  | MaX-C 11-15 Feb 2019 | Casalecchio (IT) | Carlo Cavazzoni   |
| Towards Reality in Nanoscale Materials X  | MaX-C 12 Feb 2019    | Levi (FI)        | Zeila Zanolli (Invited Talk)  |

|  |                      |                |   |
|--|----------------------|----------------|---|
| FocusCoE Workshop  | MaX-C 21 Feb 2019    | Frankfurt (DE) | Elisa Molinari, Luisa Neri, Silvana Muscella, Francesco Osimanti  |
| Materials and Scientists of the Future: the Space Girls visiting MaX CoE       | MaX-E 5 Mar 2019     | Lausanne (CH)  | Elisa Molinari  |
| AiiDA plugins migration workshop   | MaX-E 25-29 Mar 2019 | Lausanne (CH)  | EPFL Team (Giovanni Pizzi, Leopold Talirz, Elsa Passaro)  |
| EOSC-hub Week 2019   | MaX-C 9-12 Apr 2019  | Prague (CZ)    | Giovanni Pizzi  |
| EMMC expert meeting on business aspects of materials modelling marketplaces    | MaX-C 7 May 2019     | Lausanne (CH)  | Nicola Marzari  |
| Lavoisier Discussion on Quantum Simulation                                     | MaX-C 8-9 May 2019   | Barcelona (ES) | Zeila Zanolli, Nicola Marzari, Daniele Varsano, Pablo Ordejon   |
| European HPC Summit Week 2019  | MaX-C 13-17 May 2019 | Poznan (PL)    | Fabrizio Magugliani, Carlo Cavazzoni (giving a talk @ EuroHPC co-design workshop), Sebastiaan Huber (EPFL, talk ), Elisa Molinari and Luisa Neri (CNR Nano)             |
| Tutorial on writing reproducible workflows for computational materials science | MaX-T 21-24 May 2019 | Lausanne (CH)  | Giovanni Pizzi, Leopold Talirz, Spyros Zoupanos, Sebastiaan Huber, Nicola marzari (EPFL); Andrea Ferretti (CNR Nano); Stefaan Cottenier (UGent); Alberto Garcia (ICMAB) |
| HPC for Industry 4.0   | MaX-C 21-23 May 2019 | Milano (IT)    | Elisa Molinari, Fabrizio Magugliani   |
| NanoInnovation 2019  | MaX-C 11-14 Jun 2019 | Rome (IT)      | Mariella Ippolito   |
| PASC19   | MaX-C 12-14 Jun 2019 | Zurich (CZ)    | Zeila Zanolli - Carlo Cavazzoni   |



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|  |                      |                     |   |
|--|----------------------|---------------------|---|
| ISC2019  | MaX-C 16-20 Jun 2019 | Frankfurt (DE)      | Fabrizio Magugliani   |
| Advanced School on Quantum Transport with SIESTA       | MaX-T 23-29 Mar 2020 | Donostia (ES)       | The QUANTUM ESPRESSO Foundation and the EU MaX Centre of Excellence for Supercomputing Applications |
| Picking flowers: Hands-on FLEUR                        | MaX-T 9-13 Sep 2019  | Juelich (DE)        | Daniel Wortmann, Stephan Bluegel  |
| Quantum Espresso Summer School                         | MaX-T 16-20 Sep 2019 | Ljubljana, Slovenia | Attendees to be defined   |
| MaX-Graphene Flagship joint event @ Graphene Week 2019 | MaX-E 23-27 Sep 2019 | Helsinki (FI)       | Attendees to be defined   |
| European Research and Innovation Days                  | MaX-C 24-26 Sep 2019 | Brussels (BE)       | Attendees to be defined   |