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D7.3 – Communication, dissemination, and stakeholders engagement strategy and plan

Version 1.0

GA no 952165

Dissemination Level

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	PP: Restricted to other programme participants (including the Commission)
	RE: Restricted to a group specified by the consortium (including the Commission)
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Abbreviations

Abbreviation	Translation
AiiDA	AUTOMATED INTERACTIVE INFRASTRUCTURE AND DATABASE FOR COMPUTATIONAL SCIENCE
CINECA	CINECA CONSORZIO INTERUNIVERSITARIO
CoE	CENTRE OF EXCELLENCE
CNRS	CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE CNRS
HiPEAC	EUROPEAN NETWORK ON HIGH-PERFORMANCE EMBEDDED ARCHITECTURE AND COMPILATION
HPC	HIGH PERFORMANCE COMPUTING
KER	KEY EXPLOITABLE RESULTS
KTH	ROYAL INSTITUTE OF TECHNOLOGY
MaX	MATERIALS DESIGN AT THE EXASCALE
Megware	MEGWARE COMPUTER VERTRIEB UND SERVICE GMBH
MPG	MAX-PLANCK-GESELLSCHARFT ZUR FORDERUNG DER WISSENSCHAFTERN EV
NCC	NATIONAL COMPETENCE CENTRE (FOR HPC)
QMC	QUANTUM MONTE CARLO
R&D	RESEARCH AND DEVELOPMENT
SISSA	SCUOLA INTERNAZIONALE SUPERIORE DI STUDI AVANZATI DI TRIESTE
STUBA	SLOVENSKA TECHNICKA UNIVERZITA V BRATISLAVE
TREX	TARGETING REAL CHEMICAL ACCURACY AT THE EXASCALE
TRUST-IT	TRUST-IT SRL
TUL	POLITECHNIKA LODZKA
UNIVIE	UNIVERSITAT WIEN
UT	UNIVERSITEIT TWENTE
UVSQ	UNIVERSITE DE VERSAILLES SAINT-QUENTIN-EN-YVELINES

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Executive Summary

The main goal of the TREX Centre of Excellence (CoE) is to enable the community codes for stochastic quantum chemical simulations to successfully exploit the most advanced European computing facilities, i.e., the EuroHPC pre-exascale and exascale machines, and foster the use of supercomputers with energy-efficient accelerators (e.g., GPU) by means of state-of-the-art quantum Monte Carlo (QMC) codes, developed in Europe and internationally recognised as key algorithmic assets. This will be achieved via a co-design approach to the development of the QMC community codes in order to prepare them for the next generations of HPC hardware.

In line with this goal, this document sets out an effective communication, dissemination and stakeholders engagement strategy to be implemented by the consortium during the 36 months of the project. Consistent and content-rich communication is strategic to showcase the results and impact of the TREX project. This plan has been built on a continuous set of actions of communication and dissemination campaigns for the main TREX assets, primarily the TREX community codes for advanced QMC simulations, complex scalable workflow, and training and educational activities, ensuring coverage of all stakeholders and adequate visibility worldwide. The custom-made TREX web web-platform is at the heart of the engagement, outreach and exploration strategy of the project, it is the technological engine behind the technical support to end-users of TREX software, hands-on workshops to forge a new generation of code developers.

Various communication and promotional campaigns are presented in this document, with detailed timelines presenting the activities that will be put in place. For each of these campaigns, specific communication, dissemination, and stakeholder engagement activities and synergies within the EU HPC ecosystem are detailed to ensure the successful achievements of the project objectives.

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1 Introduction

1.1 Purpose and Scope

The main purpose of this deliverable is to define the continuous set of actions of communication and dissemination and stakeholder engagement strategy for the 36-month TREX innovation activities.

This report will have two more releases, due in March 2022 (M18) – *D7.4 "Communication, dissemination, and stakeholder's engagement interim report*, and user uptake updates, and in September 2023 (M36) – *D7.6 "Communication, dissemination, and stakeholder's engagement final report*.

These future iterations will build on this first version, outlining also the activities on work package (WP) six (WP6) – Training and user uptake, which started in October 2020. The WP6 coordinates the structured training and educational activities of TREX. These cover technical support to end-users of TREX software, hands-on training for code users in academia and industry, and hands-on workshops to forge a new generation of code developers. Special attention is given to the engagement of communities within the European countries that are currently developing their HPC ecosystem. WP6 will also target the education of young pupils and university students by developing a visual and modular tool for stochastic quantum simulations as well as coupling a yearly satellite event to a wide European school for master students.

Also, this plan is drawing on T8.3 – Coordination with initiatives in the HPC materials ecosystem (UT), which started in October 2020 (under WP8 – Project Management, Coordination and Sustainability) and which is zooming in on the synergy aspects, and initiatives in the HPC ecosystem, particularly with the other HPC Centres of Excellence. The coordination activity thus creates a direct link with the uptake outreach activities in a pan-European arena, including CoE governance structure and associated infrastructure, as well as the project operational guidelines, as reported on D8.1 "Project Handbook" due in March 2021 (M6).

1.2 Structure of the document

The document is leanly structured in seven sections:

- Section 1: outlines the purpose, structure of the document and its relation to other TREX documents.
- Section 2: presents the project communication and stakeholder engagement strategy, and illustrates the TREX target stakeholder's group, with clear benefits for them in engaging with the project.
- Section 3: describes the key expected project results and assets.
- Section 4: brings us within the core communication, dissemination activities with details on the overall communication and engagement tools and channels to be used to make the plan as pragmatic as possible, including online presence and content production, collaterals and social media channel utilisation and distribution.
- Section 5: offers a list of training and educational activities and plans for the next 18 months of the project.
- Section 6: continues with an overview of TREX organisation and participation in events.
- Section 7: presents the KPIs monitoring activities and the impact, including the online dashboard monitoring the visibility, engagement, and dissemination potential of online activities in automated software that will be used throughout the entire project duration.

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1.3 Relation with other documents

WP7 keeps track of all deliverables closely related to communication, dissemination and stakeholder engagement uptakes:

- D7.1 TREX branding and communication kit, Nov 2020 (M2) – Trust-IT
- D7.2 TREX Web platform, Jan 2021 (M3) – Trust-IT
- D6.1 TREX Training and Education Strategy and Plan, with subsequent updates, Jan 2021 (M3) - STUBA
- D7.3 Communication, Dissemination, and Stakeholders-Engagement Strategy and Plan, Mar 2021 (M6) – Trust-IT
- D8.1 Project Handbook, including CoE governance structure and associated infrastructure as well as operational guidelines, Mar 2021 (M6) - UT
- D7.4 Communication, Dissemination and Stakeholders Engagement Interim Report, and user uptake updates, Mar 2022 (M18) – Trust-IT
- D6.2 First report on the status of organisation of training events and activities, including validation surveys, May 2022 (M20) - STUBA
- D7.5 TREX Blueprint distributed at TREX Final-Results-Oriented Event, Jul 2023 (M34) – Trust-IT
- D7.6 Communication, Dissemination and Stakeholders-Engagement Final Report, Sep 2023 (M36) – Trust-IT

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2 The TREX Communication and stakeholder engagement plan

TREX will execute a coordinated 36-month communication and stakeholder strategy covering the design set-up and management of 1) the TREX web-platform, 2) dissemination of TREX Key Exploitable Results (KERs)1, namely software, codes and libraries, 3) ensuring visibility of TREX demonstrators, 4) reaching out to relevant communities interested in TREX assets and codes, and 5) providing support to the training for higher education and industry. These represent the key pillars of the TREX communication and stakeholder engagement campaigns (Figure 1).

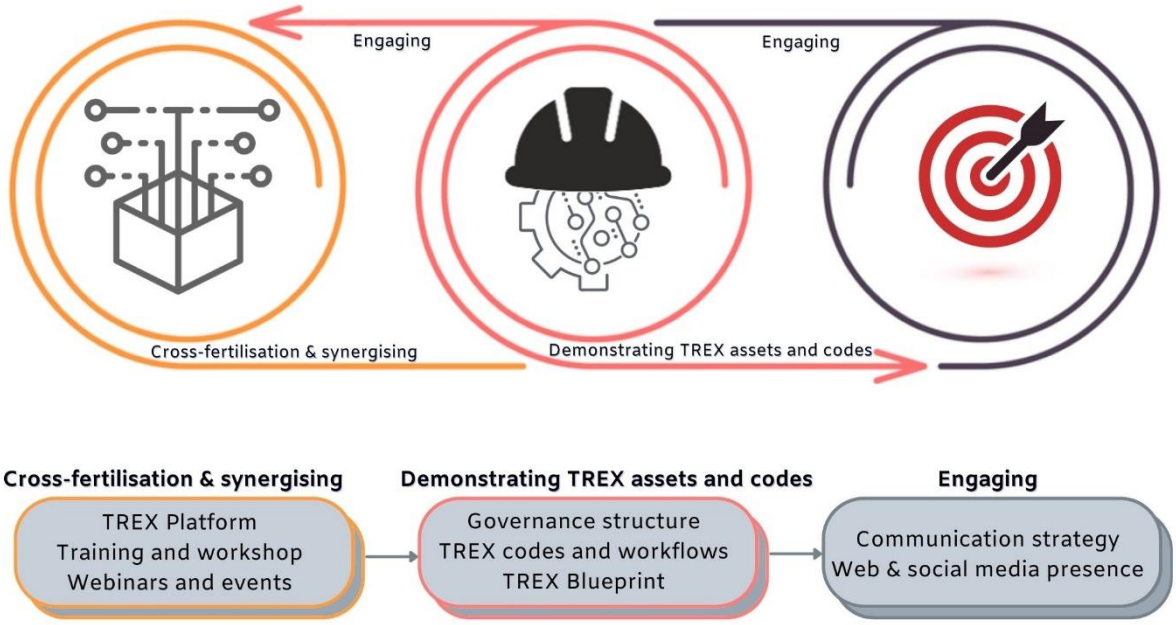

Figure 1: TREX Communication pillars

1. **TREX platform as a sustainable asset**. The platform (website) acts as a Single-Entry Point to access the vast majority of the results, the dissemination activities, the training material as well as general information and resources like branding elements, news, and events, including training modules. All partners are expected to contribute, providing proof of user uptake with strong user benefit awareness.
2. **TREX software, codes and libraries**. Visibility and access to the TREX codes, libraries and software, will be ensured particularly via the TREX website where, e.g., links will guide visitors to repositories for TREX codes. Training and informative material will be provided, too, accompanying the descriptions of these Key Exploitable Results (KERs).
3. **Ensuring visibility to TREX Demonstrators.** Specific actions will be undertaken to ensure visibility to the challenging exascale-enabled demonstrations that will be designed by TREX to test the readiness and effectiveness of TREX software into real exascale use cases, namely

[1] According to the Horizon 2020, a result is defined as: "*Any tangible or intangible output of the action, such as data, knowledge and information whatever their form or nature, whether or not they can be protected, which are generated in the action as well as any attached rights, including intellectual property rights*". A Key Exploitable Result (KER) is an identified main interesting result (as defined above) which has been selected and prioritised due to its high potential to be "exploited" – meaning to make use and derive benefits - downstream the value chain of a product, process or solution, or act as an important input to policy, further research or education.

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those identified in the field of materials for energy conversion; water description; quantum magnetism and high-temperature superconductor and functional materials

4. **Reaching out to the relevant communities**. Potential stakeholders from a diversity of groups will be approached through targeted campaigns and communication instruments, ranging from news articles, social media outreach, and events to webinars, newsletters, interviews, and videos.
5. **Training for higher education and industry**. Capacity building and training events, including hands-on workshops, satellite events, and the final school, both for academia and industry to create awareness on TREX assets and the demonstrations led by WP5.

Last but not least, the TREX Blueprint will also tackle the results of the outreach campaigns performed towards the assets mentioned above with an indication of the main recommendations tacking user uptake and exploitation of TREX Key Exploitable Results (KER).
The associated campaign will be implemented via a series of communication and dissemination activities that are detailed in Section 4 of this document.

The dissemination, communication and stakeholder engagement plan is managed in WP7, which has a role in the project in terms of communicating and disseminating Key Results to target stakeholders (Figure 2).

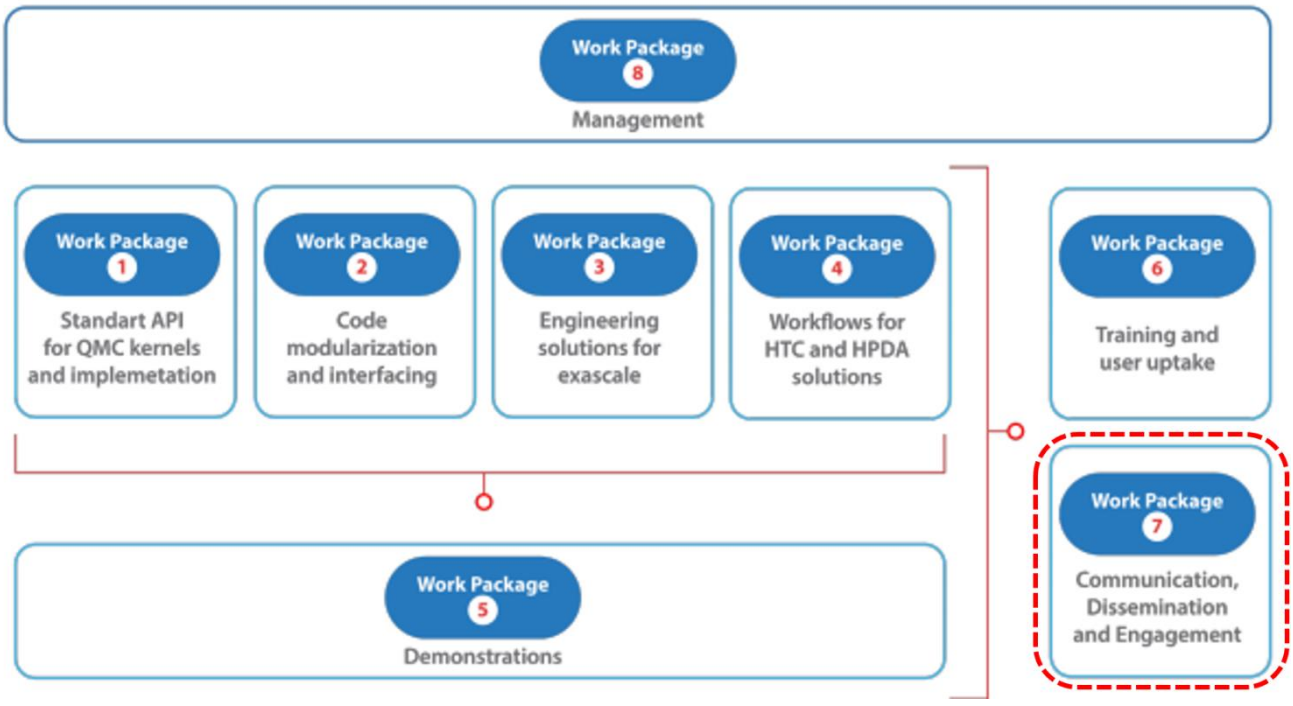

Figure 2: Positioning of WP7 in TREX

Input for WP7 activities will come from all other WPs:

- WP1 – Standard API for QMC kernels and implementation (CNRS)
  - Establishing common design principles and developing an **easy-to-read and easy-to-modify library,** enabling the **wide community of QMC experts, code owners, and newcomers.**
- WP2 – Code modularisation and interfacing (SISSA)
  - Presenting **flagship codes platform** to users and developers, in order to seamlessly integrate their unique capabilities within an interoperable framework.
- WP3 – Engineering solutions for exascale (KTH)
  - Benchmarking and profiling the TREX software activities with respect to different hardware features, providing **high-performance implementations of TREX codes** for upcoming supercomputers in co-design with the HPC partners.
- WP4 – Workflows for HTC and HPDA solutions, algorithms, and toolkits (UNIVIE)
  - Developing robust workflows to enable **users to easily perform standardised QMC calculations, operate TREX codes in a pipeline, and work in high-throughput computing (HTC) fashion** when using exascale resources for machine learning purpose.
  - Helping HPC centres to go beyond their traditional usage models by advancing, provisioning e-infrastructure services such that new **workflows for the QMC community are realised.**
- WP5 – Demonstrations (CNRS)
  - Providing **invaluable feedback** in terms of testing and demonstrating the **effectiveness of TREX software**.
- WP6 – Training and user uptake (STUBA)
  - Coordinating and structuring training and educational activities of TREX. These cover technical support to end-users of TREX software, hands-on training for code users in academia and industry, and hands-on workshop to forge a new generation of code developers. Targeting young pupils and university students by developing a visual and modular tool for stochastic quantum simulations, as well as coupling a yearly satellite event to an established European school for master students.

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2.1 Objectives

The specific objectives of this plan for communication and stakeholder engagement and promotion of the TREX activities, results and impacts are summarised in Table 1.

Table 1: TREX communication goals

Objectives	Main Target Activities
Implementing a multi-stakeholder engagement plan	• Guarantee sharing of information and engagement via webinars and events; • Establish key strategic partnerships with the HPC ecosystem, leveraging on the synergy with the HPC CoEs; • Producing regular, focused, and high-quality content on core project activities; • Design and maintain an editorial plan including all relevant communications material and channels;
Showcasing TREX results, creating awareness of the QMC community codes and libraries.	• Developed and continuously evolved to be the Single-Entry Point for all the results and outcomes of the project; • User-friendly documentation for the use of TREX software components (libraries and codes); • Creation of webinars and workshops with high-profile experts in the HPC domain.
Ensure global recognition and visibility on how the QMC community codes are pursuing world-class innovation	• Support the collaboration and partnership with other HPC CoEs; • Create a lasting legacy community of HPC experts in QMC and engaged actors within the HPC ecosystem and within other communities (e.g., CECAM, MaX, PoP, PRACE, Fenix, EuroHPC Joint Undertaking), as well as the needs of the user communities to reach the targeted users and other stakeholders.
Ensuring a proper branding strategy and recognition	• Equip all partners with information and marketing materials for outreach purposes to the specific target audience; • Supporting consensus building and raising awareness on the progress of TREX also in building an international community covering all stakeholders playing a role within the TREX ecosystem, including universities and research institutes, owners of codes, policymakers/national funding agencies, regulators, standards bodies and national governments etc. • Ensure alignment and collaboration with the H2020 HPC CoEs, HPC communities (and pan-European initiatives.

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2.2 TREX value proposition

With the continuous evolution in technology, TREX will address three main challenges faced by different target stakeholders, see Figure 3.

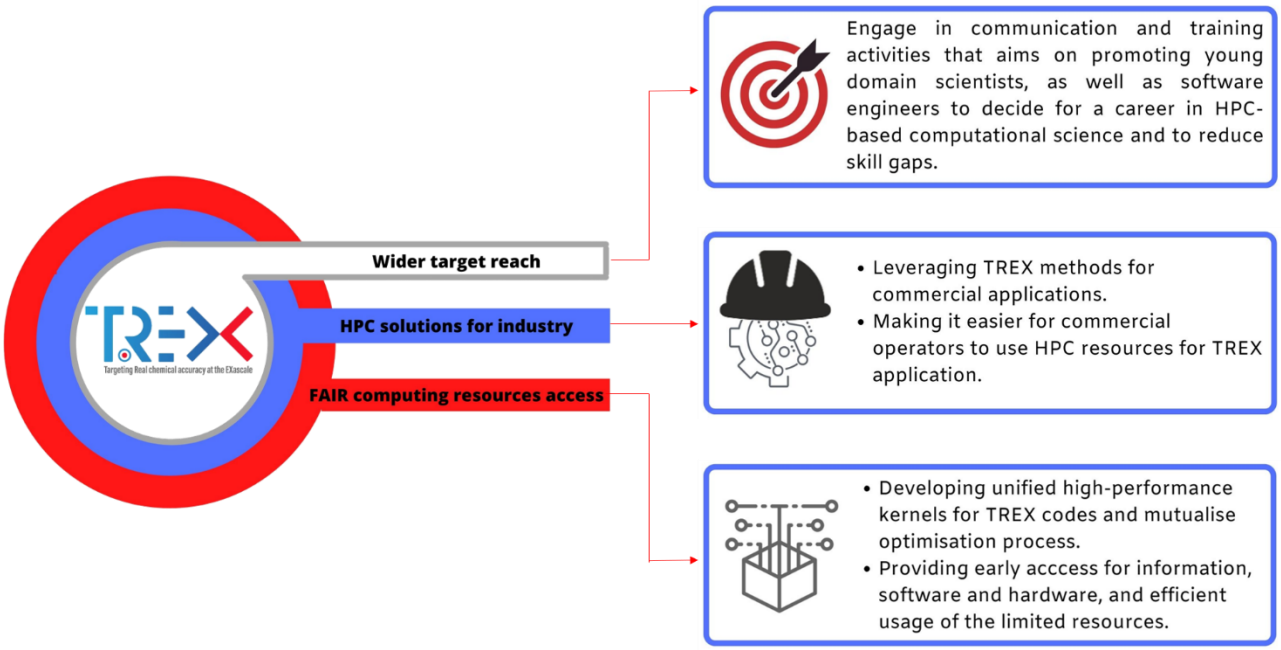

Figure 3: TREX Value Proposition

2.3 TREX Stakeholders

One of the main objectives of the TREX dissemination and exploitation strategy is to ensure that TREX codes are usable and used by the identified target groups from the academic and non-academic sector.

Current and upcoming players in the European HPC ecosystem (external to TREX), including Undergraduate and PhD students, postdocs, and researchers and trainers. TREX is aiming at enlarging the uptake of domain-specific and HPC applications in Europe in particular by the new **generation of Computational Science researchers** TREX exploitation strategy will therefore closely align with the EuroHPC strategy towards improving the uptake of HPC resources. **Training** will be at the core of this engagement via the organization of **webinars, lectures, videos** as well as the production of extended technical and co-design documentation that will become available via the TREX website. TREX will seek coordination with other CoEs (in particular, MaX and MARVEL), NCCs, and organisations (e.g., PRACE) on HPC and exascale computing so as to ensure cross-fertilisation with the user community. The **hands-on workshops and schools** for users and developers will be a key channel to reach this target audience.

Current and upcoming players beyond the European HPC ecosystem. The technical challenges tackled by TREX both in quantum simulations and in HPC are also worked on by a worldwide scientific community and in particular by the Chemistry community. Significant efforts are ongoing to enable such simulations for upcoming exascale systems. For instance, in the US the QMC application QMCPACK is part of the Early Science Program for Aurora, which is an exascale system that is being built at Argonne National Lab.

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Liaisons with be established in particular with HiPEAC, the European network of world-class computing systems researchers, industry representatives and students, and PSNC, or the Institute of Bioorganic Chemistry of the Polish Academy of Sciences

Hardware manufacturers and industrial players (internal and external to TREX). The results of our detailed performance assessment of TREX codes and TREX library will be potentially shared with industrial stakeholders, including providers of HPC solutions (including hardware) and those companies that are interested in QMC simulations for their R&D. For the latter category, this may constitute the basis for collaboration related to hardware and/or software improvements (compiler/OS) to be eventually driven by **hands-on workshops**. Also, **training** will be organised on specific use cases of relevance to these target stakeholders, while **technical documentation** or specific, **industrial sessions** as part of other end users' **events** will be exploited as much as possible. **Use cases** from the industry sectors will be produced and promoted via TREX communication channels, leveraging **testimonials and interviews** as a marketing lever.

Sample of industrial stakeholders include: Sipearl, Atos, AMD and ARM as well as all those companies that use TREX HPC codes for their R&D.

Policy stakeholders, including agencies, and national authorities. This category will be the target audience for the final event with the aim of ensuring awareness and uptake of the TREX recommendations. The core vehicle of the training towards policy stakeholders will be the TREX Blueprint containing a set of key recommendations to advise them on which priorities, challenges, and gaps can be further addressed under EuroHPC, Horizon Europe and Digital Europe Programmes. The Blueprint will be based on **consultations** resulting from TREX interactions with architects and integrators at HPC centres as well as other HPC players at existing CoEs. Continuous production of regular, focused, and high-quality **content** on core project activities will contribute to raising awareness on the progress of TREX towards policy stakeholders.

With the evolution of HPC architectures and software, it is important for TREX project to collaborate and foster a productive relation with key HPC players of the European initiatives such as HPC ecosystems, HPC CoEs, chemistry and domains-specific actors and industry. The first six months have seen an active participation of TREX in a broad number of collaborative events and meetings contributing to the HPC CoE mission.

The Project Handbook D8.1 provides details on the CoE governance structure and associated infrastructure as well as the project operational guidelines. The management activities will be monitored within Work Package 8 “Project Management, Coordination and Sustainability”. The Handbook is a dynamic document and will be updated as required throughout the project.

All actions described above cannot be achieved without the engagement of the scientific users communities and the strong commitment of TREX partners to enlarge the pool of users and developers in domain-specific and HPC applications.

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In addition, direct interactions have been established with other HPC CoEs whose domain is most closely related to TREX with discussions and plans for some joint activities, as well as participating in several chemistry and domain-specific initiatives, events such as:

HPC CoE events:

- FocusCoE Centres of Excellence Webinar: Interaction with Industry and SMEs[2] – 27 November – 4 December 2020
- Co-Design Workshop[3] – 12 March 2021
- 3rd EMMC International Workshop 2021[4] – 2-4 March 2021
- EuroHPC Summit Week 2021[5] – 22-26 March 2021

Chemistry and domain specific training and events:

- Tuning Workshop, Vi-HPS[6] – 7-11 December 2020
- Lucheon Winter School - TREX Tutorials in QMC[7] – 25 January – 8 February 2021
- Helmholtz GPU Hackathon 2021 - Digital Event[8] – 15-24 March 2021

[2] https://trex-coe.eu/events/focuscoe-centres-excellence-webinar-interaction-industry-and-sme
[3] https://trex-coe.eu/events/coes-co-design-workshop
[4] https://trex-coe.eu/events/3rd-emmc-international-workshop-2021
[5] https://trex-coe.eu/events/eurohpc-summit-week-2021
[6] https://trex-coe.eu/events/tuning-workshop-vi-hps
[7] https://trex-coe.eu/events/luchon-winter-school
[8] https://trex-coe.eu/events/helmholtz-gpu-hackathon-2021-digital-event

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3 TREX results and assets

The following sections provide an overview of the main assets of the project that will be at the core of this communication, dissemination and engagement plan, with initial indications on the main channels and tools to be exploited to ensure proper visibility.

3.1 Software platform & services

The **TREX consortium** is committed to building an efficient and state-of-the-art framework in HPC and exascale computing by developing an integrated **software** platform. The main goal is to provide a sophisticated computational facility of software and services for the exploitation of the new **EuroHPC supercomputers**, to facilitate stochastic quantum chemical simulations, and to enable scientific and industrial stakeholders to benefit from these large-scale machines.

The **TREX website** will be the entry point for the HPC assets and **Key Exploitable Results (KERs)** developed by the consortium, therefore a specific area will be dedicated to TREX software platforms and services with great visibility ensured already from the homepage.

- At the centre of the website offer, there will be the **TREX quantum Monte Carlo (QMC) flagship codes**, offered to the TREX stakeholders as a unique possibility to compute high-accuracy properties for very large or extended systems, where other accurate quantum chemical approaches are often very difficult to apply.
- The TREX website will also grant users and developers access to the **integrated and high-performance platform of independent codes**, a flexible, open, and inclusive platform for software development, which will act as a reference centre for all the communities in quantum chemical simulations at the exascale.
- The high-performance self-standing QMC kernel libraries will be an asset to be included in this area. Since all the software produced by the TREX project in terms of repositories and codes will follow an open-source development model, specific reference to the BSD license will be ensured, facilitate their introduction in commercial codes, and allow private companies to provide revised versions to the final users, see Figure 4 and Figure 5.
- Finally, a **software repository area** will link to those repositories where the TREX Consortium's academics and experts have decided to host and share their code development work (GitHub).

Dedicated pages and specific dissemination materials (information factsheets) will be produced about each of the above-mentioned assets, while interviews with consortium members will be an important channel to ensure an easier flow of information.

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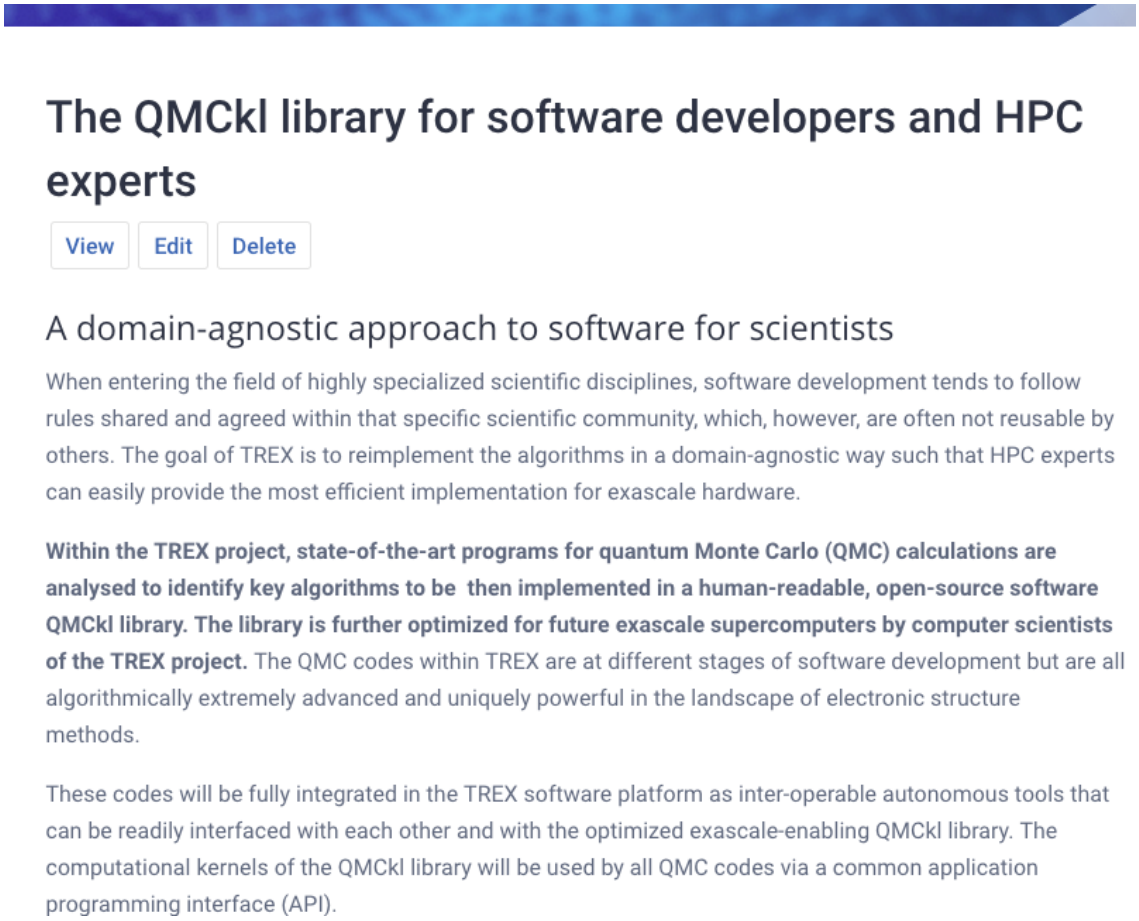

Figure 4 Sample webpage dedicated to TREX QMC kernel libraries available at https://trex-coe.eu/qmckl-library-software-developers-and-hpc-experts-0

Figure 5 Video interview with Anthony Scemama introducing the TREX QMCKl library, available at https://youtu.be/HIXMTnBMnIc

TREX strongly pursues synergy and complementarity with existing CoEs. We will adopt the AiiDA[9] Materials Informatics Framework and the Materials Cloud Archive of MaX CoE for workflow management and HTC, and data analysis as well as the Scalasca and MAQAO tools of POP CoE for software performance analysis and optimization. Furthermore, TREX will join the efforts of initiatives such as FocusCoE[10] for the coordinated action enabling CoEs to more effectively fulfil their role within the HPC ecosystem.

TREX will provide benchmarks to validate the use of appropriate functionals for specific problems to further promote the established role of QMC as a source of information for improving or devising functionals; develop interfaces to share the respective expertise, entailing an enriched toolbox for quantum mechanical modelling of materials, with European added value. TREX is endorsed by MaX[11] Coordinator (Prof. Elisa Molinari) and MaX member and director of NCCR MARVEL[12] (Prof. Nicola Marzari): they both envision close collaboration on the abovementioned developments (see support letters).

3.2 Demonstrators

Specific communication campaigns will be designed and implemented to ensure visibility to the challenging exascale-enabled demonstrations that will be designed by TREX to test the readiness and effectiveness of TREX software into real exascale use cases, namely those identified in the field of materials for energy conversion; water description; quantum magnetism and high-temperature superconductor and functional materials.

Demo 1 Materials for energy conversion. This demo will explore exciton physics in two-dimensional (2D) materials, expected to become active building- blocks in future optoelectronics. QMC simulations of representative 2D nanomaterials (e.g., free-standing fluorographene) will be performed, scaling to unprecedented models' sizes (~2,000 electrons), that enable the presence of the exciton in its full size.

Demo 2 Accurate and reliable description of water. Study the complex interactions which take place in water and govern all its phases is not a simple endeavour: the number of possible minima grows combinatorically with the size of the cluster model and their relative energetics must be accurately predicted for the quantitative treatment of aqueous solvation of ions or molecules. The exascale-enabled TREX software will provide unprecedentedly accurate data for many and large water clusters and solutes, presently too expensive for traditional highly-correlated methods.

Demo 3 Microscopic description of quantum magnetism and high-temperature superconductors. Low-lying spin states in quantum chemistry and competing magnetic phases in condensed matter are both footprints of strong electron correlation. It is extremely challenging to describe the spin and oxidation states of the open-shell transition metal atoms in complexes such as the oxygen-evolution complex (OEC) for water splitting in Photosystem II or the FeMoCo cofactor for nitrogen fixation in Nitrogenase. Using FCIQMC methods with their accurate account of both dynamical and static correlation, TREX will compute various spin states and determine the spin ladders of the OEC and

[9] https://www.aiida.net/
[10] https://www.hpccoe.eu/about/
[11] http://max-centre.eu/
[12] https://nccr-marvel.ch/

FeMoCo complexes. This demonstration will apply large scale active space methods, followed by dynamical correlations using externally corrected Coupled-Cluster. At the same time, HPC-enabled QMC method will tackle the study of the phase diagram of high-temperature superconductors, whose mechanism is still debated and where a proper description of magnetic order is important.

Demo 4 Van der Waals functional materials: strained and excited beyond-graphene systems. Van der Waals interactions are ubiquitous and play a key role in layered materials, which bear high promise for fast, dissipationless, flexible next-generation electronic devices. This demonstration will focus on graphene and beyond- graphene (such as borophene) clusters, including monoelemental and single-sided halogenated bi-layer structures, poorly understood in strained or electronically excited configurations.

Sample activities includes **demonstration sections on the TREX website**, with single pages dedicated to each demonstration with informative materials and available documentation and dedicated **branding materials** spamming icons and images, see Figure 6. A categorisation can be implemented, too, with filters and labels guiding users to find the demonstrations that best match their needs. The area will also constitute the main entry point to access the supercomputing resources needed to execute the demonstrations by new users. **Factsheets and videos** will be produced, while dedicated engagement activities – such as **webinars** - will be performed with projects, institutions and networks in thematic communities addressed by the demonstrators. **Interviews with the demonstration coordinators** – video, written or as podcasts – will be distributed, too.

Figure 6 TREX website area dedicated to the demonstrations

3.3 Community involvement

TREX will offer technical support to the users through the adoption of a single point of contact (SPC) offered via the main TREX website. This will consist of an online form and an email address to which all the request for assistance will be conveyed.

The TREX **help desk** will also serve as an online engagement tool. An online **support triage** will be set up via the website to ensure the support request is referred to the correct person. At the time of writing this deliverable, the following options are being discussed:

- the usage of a trouble ticketing system (such as JIRA) directly accessible via the website, allowing users to open ticket autonomously; this can also be moderated by a support triage team to be contacted by users via a contact email;
- the usage of a forum-like tool to be integrated on the TREX website, where to organise questions and topics of discussion.

The usage of simple **contact forms** is also included in this strategy.

TREX: Targeting Real Chemical Accuracy at the Exascale project has received funding from the European Union Horizon 2020 research and innovation programme under Grant Agreement No. 952165.

4 Communication and dissemination plan

Communication is a very significant factor in the success of the TREX project, by promoting and ensuring its visibility in both online and offline channels, building the TREX brand through coordinated marketing, dissemination and engagement strategy. The TREX team will work continuously to enhance the existing communication strategy in key elements such as branding visibility, exploitation of media channels, and a widened audience together. This will go hand-in-hand with the development of synergies, both internally and externally, for the overall success of the project.

This section provides an outline of the communication, dissemination, marketing and stakeholder engagement with plans on how to engage and communicate with them and includes associated KPIs for monitoring the activities and the impact.

4.1 Visual Identity and branding

A consistent visual identity will be created to back up all communication and dissemination activities. Templates for external communication and documents will also be provided. With this solid branding strategy, the project aims to achieve the following outcomes:

- Acknowledgement across a broad range of stakeholders;
- Gain trust and loyalty from the audience;
- Sustained the overall message that TREX wants to convey across the main communication sources and elements such as:
  - Website
  - Social media channels
  - Interviews and /or audio visuals
  - Marketing materials (flyers, banners, posters)
  - Press Releases
  - Impact reports

The first way to communicate about the project is the identification of the project logo. The TREX logo (Figure 7), undergone a meticulous process in order to provide an adequate *"look-and-feel"* able to suggest the involvement of the project with the Quantum Chemistry domain.

Figure 7: TREX logo

Further details are incorporated into the D7.1 TREX Branding and Communication Kit document (published in November 2020).

TREX: Targeting Real Chemical Accuracy at the Exascale project has received funding from the European Union Horizon 2020 research and innovation programme under Grant Agreement No. 952165.

Dedicated collaterals such as flyers, posters, one-pagers, cards, etc. along with printable materials will be produced over the course of the project, a number of flyers, posters and roll-up banners will be on purpose-designed for dissemination and, once the pandemic will be over, they will be printed and used at major events.

Graphical materials for TREX will include:

- Flyers – used mainly as a handout, they will be distributed n printed format at physical events for better user engagement.
- Posters – the main project outcomes and figures will be collected and showcased in a poster format, for quick yet comprehensive visualisation of the project.
- Roll-up banners – mainly intended for visibility at busy events, and to stand out of the crowd within project booths and desks, or as background images for footage and pictures.
- Brochures – an inclusive document in a pocket version. To be used as the main project reference, collecting all the relevant project information and outcomes.

Document templates for external communication have been set-up to guarantee a univocal communication style and provide the entire TREX's consortium with a shared toolkit of Communication tools to be utilised in a recurring situation and events, deliverables or formal exchanges to outreach specific target audience (Figure 8, Figure 9, and Figure 10). All templates will be stored and completely accessible for the Consortium members in the common repository, as described in the D8.1 Project Handbook.

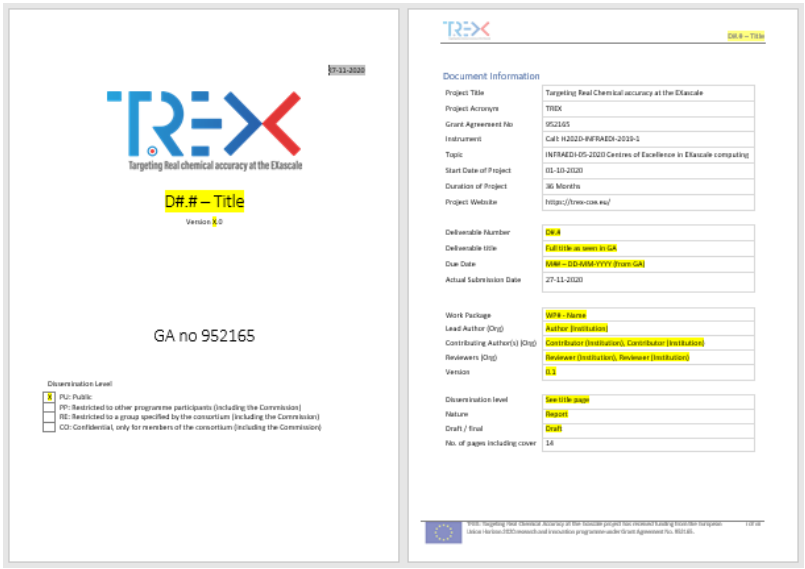

Figure 8: TREX Deliverable Template

Figure 9: TREX PowerPoint Template

Providing the research community with unique exascale computational power instruments to push quantum chemistry simulations a step further

Recently launched under the EU Horizon 2020 Research and Innovation Programme, the TREX is the new HPC Centre of Excellence for quantum chemistry. It tackles the great challenge of enhancing the tools available for the chemistry community to understand the fundamental properties of the matter.

1 October 2020

In recent years, the European Commission has seriously committed to the challenge, which also see US and China competing, to build one of the first computers able to reach the computational power of 1 Exaflop (i.e. 1'000'000'000'000'000'000 or $1x10^{18}$ operations per second!), with the establishment of the EuroHPC initiative (https://eurohpc-ju.europa.eu/). This huge computational power will permit to perform simulations which are not affordable at the moment, challenge the limits of scalability of the applications but also enable ensemble simulations in a so-called high-throughput approach (for example, screening a huge number of drugs to quickly find the most effective ones). Naturally, such investments pose a series of questions, spamming from enabling massive parallelism to tackling with heterogeneous models of supercomputing architectures. **In order to face these challenges, a huge and joint effort of domain scientists and computational experts is required.** This rationale pushed the European Union to fund targeted Center of Excellences, each supporting a specific community. **The European Center of Excellence in exascale computing TREX – Targeting Real chemical accuracy at the EXascale - falls under this remit and has officially started its activities on October 1st 2020.**

TREX: Targeting Real Chemical accuracy at the EXascale

In quantum chemistry and materials science, it is really hard to achieve exascale scaling: a large amount of electronic structure applications is still struggling to get the most out of the computational power of current software, and a lot of effort is actually put in moving towards a class of problems able to take advantage of new machines and infrastructures in the exascale era. On the other hand, quantum Monte Carlo (QMC) approaches are intrinsically parallel and they are among the few methods in the field of quantum simulations that can fully exploit the massive parallelism of the upcoming exascale architectures. The marriage of these advanced methods with exascale will enable simulations at the nanoscale of unprecedented accuracy, targeting a fully consistent description of the quantum mechanical electron problem for very large systems.

The TREX Center of Excellence (CoE) aims at developing, promoting, and maintaining open source high-performance software solutions in the field of quantum chemistry, ready to take advantage of upcoming exascale architectures. TREX gathers European scientists, High Performance Computing (HPC) stakeholders, and SMEs working on quantum chemistry simulations of extreme accuracy in the framework of stochastic Quantum Monte Carlo (QMC) methods to develop a **software solutions**

that will greatly accelerate the diffusion in academia and industry of these unique computational instruments, which have so far largely been the privy of a specialized community.
This will permit to greatly enhance the tools available to the scientific community for the design of new materials and the understanding of the fundamental properties of matter.

About the Consortium

The TREX CoE project has officially been launched under the EU H2020-INFRAEDI-05-2020 plan funded by the European Commission GA 952165.

TREX Center of Excellence is a consortium of 12 partners, universities, research institutions, and SMEs from seven different European countries, namely, University of Twente (NL), Centre National de la Recherche Scientifique (Toulouse and Paris, FR), Scuola Internazionale Superiore di Studi Avanzati (Trieste, IT), CINECA (Bologna, IT), Jülich-Supercomputing Centre (DE), Max Planck Institute for Solid State Research in Stuttgart (DE), University of Versailles Saint Quentin-en-Yvelines (FR), Megware (DE), Slovak University of Technology in Bratislava (SK), University of Vienna (AU), Lotz University of Technology (PL), and TRUST-IT (IT).
The scientific core of the consortium is closely linked to two leading European HPC Centres, that is CINECA (IT) and Jülich-Supercomputing Centre (DE), and to Megware, an SME in the field of integration of HPC solutions. Finally, the partner TRUST-IT is an SME specialized in and responsible for the communication, stakeholder engagement, and outreach activities of TREX.

For more information, visit the website https://trex-coe.eu/ and engage with the TREX platform on Twitter and LinkedIn

The TREX: Targeting Real Chemical Accuracy at the Exascale project has received funding from the European Union's Horizon 2020 - Research and innovation program - under grant agreement no. 952165.

Targeting Real Chemical Accuracy at the Exascale project has received funding from the European Union Horizon 2020 research and innovation programme under Grant Agreement **No. 952165.**

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Figure 10: Example of a branded Press Release (i.e., a signature of a Memorandum of Understanding with Small Business Standards)

4.2 TREX Web platform

The TREX website is the central communication and dissemination channel of the project. It will be hosting several project assets, which will form the website structure and are highly visible on the homepage which will be continuously evolving as the project results and assets are released or published.

Content-Driven Approach

The communication, marketing and engagement plan will concentrate its efforts on copywriting and producing engaging, stimulating and impactful content. The TREX editorial planning will include regular publication of updates covering the QMC community codes, workflows and software (contributions coming from the HPC expert partners), TREX training, workshops, webinars and events with their output, as well as other relevant events for the target stakeholders such as news pieces and interviews. Technical contents must undergo to editorial quality check prior to its publication.

4.3 Social media campaign

Social media is a core element of TREX communication, especially to follow ongoing developments and to connect to different stakeholders. TREX makes use of Social Media channels and professional networks such as Twitter (@trex_eu)[13], LinkedIn[14], YouTube[15] in order to build a stronger and highly engaged TREX community.

[13] https://twitter.com/trex_eu
[14] https://www.linkedin.com/company/trex-eu
[15] https://www.youtube.com/channel/UCgkQzeUW6O77jLpUEtm2RDA

The project is currently developing its community and initially been promoting information about TREX through its social media channels. Figure 11 are some of the top tweets and posts for the first five months of the project, garnering 2,105 impressions on the first month of the project (October 2020), and gained several top followers and influencers from the European HPC ecosystem and community, such as EOSCsecretariat.eu (@EoscSecretariat)[16], ETP4HPC (@Etp4HPC)[17] and EITCI Institute (@EITCI)[18]. **Expected KPI: 500 tweets, 100 connections on LinkedIn, and >100 non-affiliated Twitter followers by M36.**

Figure 11: TREX sample tweet and LinkedIn post

4.4 Newsletters

TREX will use the newsletter as a regular tool to inform its subscribers of the project's activities and latest QMC codes update, to engage them, and to share events and dissemination material.

The TREX newsletter will be visually appealing and align with the branding strategy. Newsletter's release will be scheduled every three months (**expected KPI: 10 release by the end of the project**), see Table 2. The issue can be increased in conjunction with specific and important events (like Webinars, Workshops or conferences) in order both to increase the enrolment of new participants or to communicate follow-up messages.

Table 2: TREX newsletter schedule

Newsletter Issue No.	Schedule Timeline/Date
Issue 1	Apr 2021
Issue 2	Jul 2021
Issue 3	Oct 2021
Issue 4	Dec 2021
Issue 5	Mar 2022

Newsletter Issue No.	Schedule Timeline/Date
Issue 6	Jun 2022
Issue 7	Sep 2022
Issue 8	Dec 2022
Issue 9	Mar 2023
Issue 10	Jun 2023

[16] https://twitter.com/EoscSecretariat
[17] https://twitter.com/Etp4HPC
[18] https://twitter.com/EITCI

4.5 Videos

As part of the communication strategy, TREX will create videos and video pills as a more impactful medium to quickly and efficiently communicate with the project audience and stakeholders.

The **video plan** will envisage the production of content to highlight expert testimonials, workshop takeaways and main results (always behind individual consent and GDPR compliant) to effectively promote the project across a wide array of media channels and to deployed in a real event as well.

All videos will be uploaded on the official TREX YouTube channel, as well as recorded webinars. The channel will be mostly used as a repository for all the project videos and will serve as a future reference for all the video material produced during the project lifespan. **Expected KPI: 3 videos over the 36-month, 200 individual views to the videos uploaded to the YouTube channel.**

Figure 12 shows some of the video interviews that were published on the TREX YouTube channel.

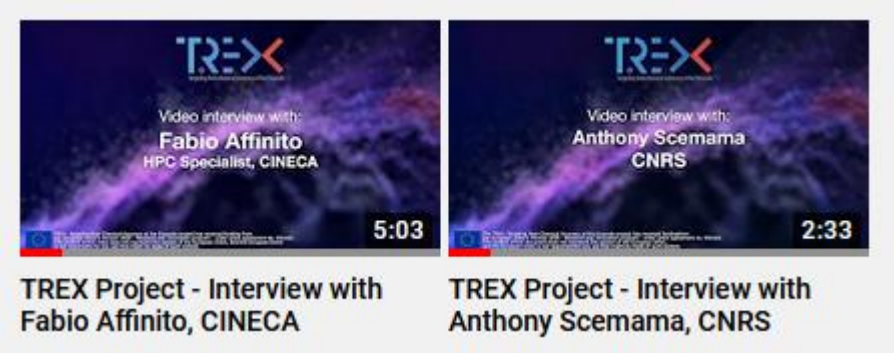

Figure 12: TREX videos

4.6 Communication tools

The communication tools aim to ensure the timely delivery of high-quality materials and tools supporting stakeholder engagement with messages tailored to various levels of knowledge. The communication tools aim to align and facilitate the engagement and communication for TREX project partners and multipliers. It is KPI-based for communications and stakeholder engagement, as described in Table 3.

Table 3: TREX engagement measure

Communication tools	KPI Description	Target KPI value over the project lifecycle
Stakeholder Database	KPI7.1 Community database	• TREX overall community (including website registrants, social media followers, participants to events and webinars) of 50 from at least 20 EU countries by M12, 150 by M24 ad up to 300 by M36.
Social media channels	KPI7.2 Social media coverage targets	• 500 tweets, 100 connections on LinkedIn, and >100 non-affiliated Twitter followers by M36; • TREX mentioned in at least 30 external social media channels by 36.
Website	KPI7.3Website targets	• For the website, it will measure the number of unique visits to main services, downloads of outputs, and site bounce rate.
Events	KPI7.4 Transfer of research results, service offers, and event-related targets	• At least 50 participants expected to attend each event ranging from policy stakeholders, students, postdocs, and researchers, industrial players, stakeholders working in public administrations; • At least 30 stakeholders reached through the TREX webinars by M36.
Videos	KPI7.5 Video production targets	• 3 videos over the 36 months; over 200 individual views of the videos uploaded to the YouTube channel.
Engagement activities (testimonials, invited talks, publications, etc.)	KPI7.6 Impact of social networking and viral marketing	• At least 10 TREX applications of industrial/technological interest; • At least 4 other quantum chemical packages integrating TREX codes; • At least 50 end-users exploiting the QMC codes; • At least 10 occasions where TREX software is used as teaching tools; • 1 final blueprint delivered to policymakers and funding agencies and downloaded by the stakeholders (reaching about 200 community members).
Content production (newsletters, news pieces and/or articles)	KPI7.7 Impacts of media outreach	• 10 newsletters circulated to subscribed community members by M36; • 12 articles by specialised and/or general media outlets by M36; • 6 content pieces published on external channels.

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4.7 Open Access Official repositories

Relying on public, open and free repositories for all the project outcomes is a pillar of the open-source strategy set in place for the project. As indicated in D7.2, the pilot use cases (demonstrations), the libraries, the flagship codes, workflows, and all algorithms, as well as the scientific publications and the project-related brand items will be publicly available through specific repositories.

On the website, all these repositories will be easily accessible via dedicated sections.

The repositories identified so far are:

- Github[19], for software components, algorithms, and libraries.
- Zenodo[20] and arXiv[21] for scientific publications; APIs will be exploited to mirror the information on the main TREX website, too.
- TREX website[22] itself, for all the collaterals, editorials and dissemination materials.

5 Training

5.1 TREX training events and workshops

Multiple training and education events open to the external audience are envisaged to take place during the TREX project lifetime. These events and actions will mostly focus on creating awareness of the TREX assets; fostering the use of the developed codes and involving future-generation of HPC ecosystems. Some of these events will be directly organised by the consortium internally, while other events will be organised by the TREX partners for external audiences. The completed plan for the training events and workshops is provided in D6.1.

5.2 Training promotion

As outlined in D6.1, the TREX website will be the main entry point for all the training materials collected and made available for the project stakeholder and external users. A dedicated training area will be easily accessible from the main homepage and will guide users, according to their profile, to training materials and information.

All necessary communication and outreach channels will be used to ensure the promotion of the training activities and engagement of target users. WP7 will provide dedicated support to ensure the promotion of the training events via all communication channels including newsletters, social media campaigns, direct email marketing and liaison with partners and multipliers (such as the FocusCOE network), as well as the dedicated training area on the project website. Target content will be produced and continuously updated, in liaison with the WP6 team and the other WPs, on the TREX website, together with news and newsletter campaigns. TREX partners and related ongoing HPC projects will ensure maximum possible resonance with the TREX training events, and additional dissemination channels like, e.g., FocusCOE initiative and related ones. TREX social media channels will also be exploited to build its community and to communicate all the training opportunities to a wide audience.

[19] https://github.com/TREX-CoE
[20] https://zenodo.org/
[21] https://arxiv.org/
[22] http://trex-coe.eu/

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6 TREX Events and Third-party events

Over its 36-month lifetime, TREX will organise three webinars and one final event to showcase all TREX results and deliver a TREX Blueprint for policymakers by the end of the project, paving the way for main recommendations for future work programme.

6.1 TREX Webinars and Podcasts

The webinar is one of the tailored disseminations and outreach activities to sensitize specific communities. A set of three (3) specific webinars will be organised and broadcasted (and eventually published for playback) to support the training elements in the other WPs showcasing the latest use cases results and impacts. This activity will be done in partnership with a technical consortium partner in order to showcase the latest TREX results.

During this time of Covid-19, podcasts are a very popular medium for learning and particularly useful as an additional communication channel that can be efficiently produced and convey information on topics of great interest in a compact medium. Podcasts may also be employed as a means of engagement to incentivise, rewarding active participation in a TREX event or workshop with increased exposure.

Engaging new software communities by inviting experts to feature on the two dissemination tools mentioned above. Both will be promoted with a news piece on the website, as well as dedicated social media posts on LinkedIn and Twitter. These social media post will also include a banner image to catch the attention of those who are scrolling through the social media feeds and create interest in viewing the whole episode, to which a YouTube link will be included in the post.

6.2 TREX Events

To maximise impact towards TREX stakeholders in collaboration with all the WPs, WP7 is promoting and supporting the organisation of EU-wide cross-dissemination & concertation, coordination meetings, webinars, workshops, training events. A regular email will be sent to the partners to gather relevant HPC-related happenings in Europe, as well as to gather meaningful takeaways from TREX members who joined any event representing the project.

WP7 is expected to organise one (**1) final event** to showcase all TREX results, and deliver a TREX Blueprint for policymakers by the end of the project and assisting WP6 in promoting the TREX training and workshops, paving the way for main recommendations for future work programme.

At the moment of writing, WP7 is assisting the WP6 in organising the first **TREX and SISSA Summer School taking place on 5-9 July 2021 in SISSA**, Trieste (IT). In preparation for the upcoming TREX event the official event page is now on-going development consisting of the following sub-pages such as programme, speakers and organisers, call for contributions and registration link, and the banner images that will be used for the dissemination and event campaign.

6.3 Other third-party events

Positioning the project inside the wide HPC ecosystems is a task that will require constant effort and engagement actions with relevant stakeholders. Among several activities that will be carried out, participation in third-party events will play a major role in the achievement of this goal. The identification and selection of key events will be regularly discussed during the monthly management meetings of the Consortium.

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Selection criteria for third-party events are HPC topics coverage, stakeholder coverage, opportunity to establish synergies with HPC and QMC-focused groups within them and/or like-minded initiatives.

An example of this type of external event is the EuroHPC Summit Week 2021, scheduled for 22-26 March 2021, and transformed into an online event in order to cope with the Covid-19 emergency. These events are still included in the TREX event section on the website tag as HPC events, in that they are not organised directly by TREX, but are pertinent to the topics address by the project.

The same communication activities will be carried out for relevant third-party events as for TREX events.

- One event news piece on the website;
- Social media posts;
- Live-tweeting at the event (*only if one of TREX partner is presenting and/or participating in the event*);
- Communication package including fliers, pop-up banner (for a physical event), and institutional presentation (*only if one of TREX partner is presenting or participating in the event*).

Table 4 is a preliminary list of the identified opportunities for the first twelve months, where TREX can look for additional visibility, a physical/virtual presence or organise co-located events.

Table 4: TREX third-party events

Event	Typology	Date, Venue
Focus CoE Centres Excellence Webinar: Interaction with Industry and SME[23]	Online event	27 Nov 2020
Tuning Workshop, Vi-HPS	Online event	7-11 Dec 2020
3rd EMMC International Workshop	Online event	2-4 Mar 2021
CoEs Co-Design Workshop	Online event	12 Mar 2021
Helmholtz GPU Hackathon 2021 - Digital Event	Online event	15-24 Mar 2021
EuroHPC Summit Week 2021	Online event	22-26 Mar 2021
GTC21	Online event	12-16 Apr 2021
ASF Roundtable	Online event	22 Apr 2021
ISC 2021	Online event	24 Jun – 2 Jul 2021
PASC21	Hybrid event	5-8 Jul 2021, Geneva, Switzerland
SC21	Hybrid event	14-19 Nov 2021, Missouri, USA

[23] https://www.hpccoe.eu/index.php/about/

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7 Monitoring activities and measuring impacts

The key strategic components of the above-mentioned communication, dissemination and stakeholder engagement strategy will be closely monitored throughout the project by meaningful measuring Key Performance Indicators (KPIs) to ensure each planned action contributes to the achievement of the project's overall goals.

The details of this approach are incorporated on D7.2. Measurable impacts will be carefully monitored via a dedicated data visualisation solution (Dashboard Analytics below in Figure 13) that will ease the analysis process while suggesting areas of improvement, as well as successful contents that need to be leveraged.

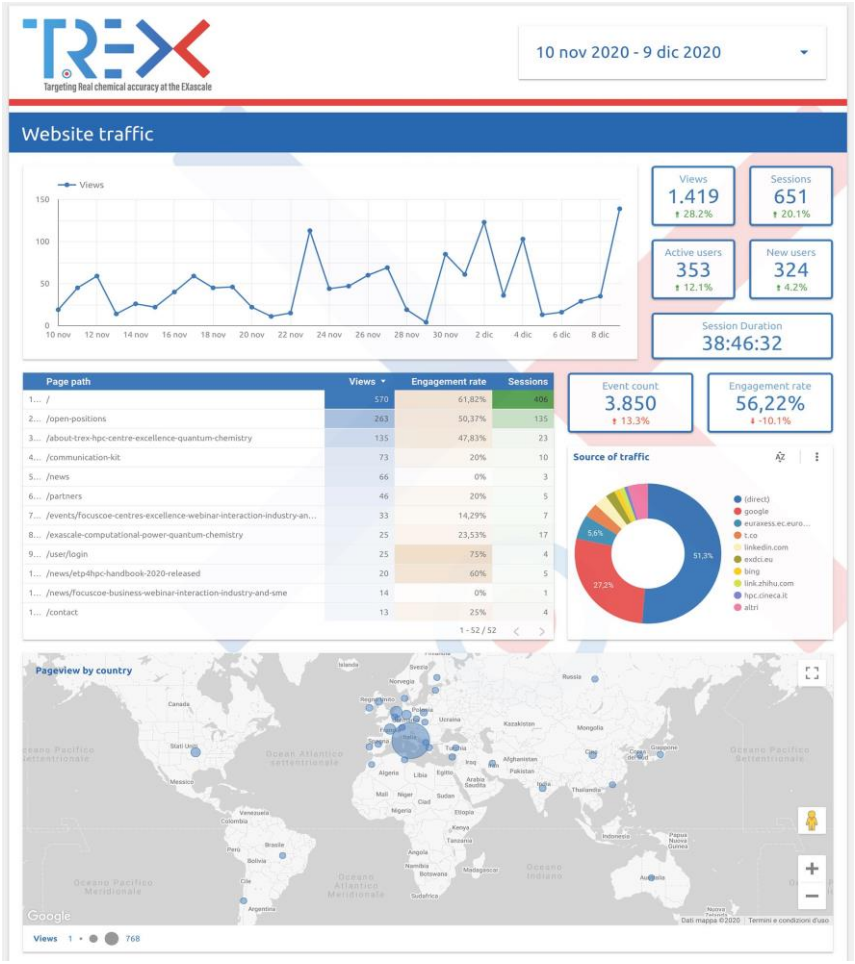

Figure 13: Illustration of the TREX Dashboard Analytical Tool

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8 Conclusion

This report is the first of a series of three reports to be produced in the course of the project. A second iteration is due in March 2022 (M18) – D7.4 "Communication, dissemination, and stakeholder's engagement interim report, and user uptake updates, and a third in September 2023 (M36) – D7.6 "Communication, dissemination, and stakeholder's engagement final report. These two other reports will analyse the results achieved in the dedicated reporting periods and will ensure updates of this plan as well as any corrective actions needed.

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