Targeting Real chemical accuracy at the EXascale

D6.1 – Training and Education Strategy and Plan

Version 1.0

GA no 952165

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	PP: Restricted to other programme participants (including the Commission)
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Abbreviations

Abbreviation	Definition
UT	UNIVERSITEIT TWENTE
CNRS	CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE CNRS
SISSA	SCUOLA INTERNAZIONALE SUPERIORE DI STUDI AVANZATI DI TRIESTE
CINECA	CINECA CONSORZIO INTERUNIVERSITARIO
FZJ	FORSCHUNGSZENTRUM JULICH GMBH
MPG	MAX-PLANCK-GESELLSCHAFT ZUR FORDERUNG DER WISSENSCHAFTEN EV
UVSQ	UNIVERSITE DE VERSAILLES SAINT-QUENTIN-EN-YVELINES.
Megware	MEGWARE COMPUTER VERTRIEB UND SERVICE GMBH
STUBA	SLOVENSKA TECHNICKA UNIVERZITA V BRATISLAVE
UNIVIE	UNIVERSITAT WIEN
TUL	POLITECHNIKA LODZKA
TRUST-IT	TRUST-IT SRL
CoE	Centre of Excellence
NCC	National Competence Centre
MaX	MAterials design at the eXascale
Marvel	National Centre of Competence in Research (NCCR) MARVEL is a centre on Computational Design and Discovery of Novel Materials created and founded by the Swiss National Science Foundation.
AiiDA	AiiDA is an open-source Python infrastructure to help with automating, managing, persisting, sharing and reproducing the complex workflows associated with modern computational science (supported by the MaX CoE and Marvel).
QMCkl	High-performance quantum Monte Carlo kernel library, one of the main outcomes of the TREX project
ML	Machine Learning
WP#	Work Package with number
SPC	Single Point of Contact
OOD	Operator-On-Duty
VI-HPS	Virtual Institute - High Productivity Supercomputing (https://www.vi-hps.org/)

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1 Introduction

The TREX Center of Excellence (CoE) aims at developing, promoting, and maintaining high-performance software solutions in the field of quantum chemistry to take advantage of the upcoming exascale architectures. The TREX software platform will enable efficient nanoscale quantum mechanical simulations of technological importance by means of advanced massively-parallel quantum Monte Carlo (QMC) methods on future-generation supercomputers. In addition to the software development, code refactoring and optimization, challenging state-of-the-art applications, including machine learning (ML) and data analytics, one of the key pillars of TREX is an outreach programme to the relevant developers' and users' communities in order to foster the use of the developed HPC codes and to engage and forge a new generation of highly-skilled computational scientists. Within the TREX proposal, this is addressed in two specific work packages (WPs) focused on training, education and user's uptake (WP6) and dissemination (WP7). The present document (D6.1 "*Training and Education Strategy and Plan*") provides an overview of the training and education programme of the TREX consortium project, as planned within WP6.

Owing to the ambitious goals and diversity of the project, the TREX training and education strategy requires several levels of approach and different groups of instructors and learners. The rich and balanced TREX training and education programme thus consists of several training events and actions and education efforts. Examples include hands-on workshops for code users and developers, schools, satellite events, hackathons, webinars, large final school and more. Direct ongoing support for the code users and developers is planned as well. The education activities include university education, hosting students and researchers, mentoring, specific training and education events, etc. Timewise, where possible, the events are ordered in an increasing-level-of-sophistication sequence (e.g., hackathons will take place in the following topic-order: programming, performance, scalability, and demonstrations). On the audience side, we focus on users as well as developers with expertise levels ranging from master students to senior researchers, in academia and industry alike. In designing the TREX training strategy, special attention is given to the engagement of communities in countries currently developing their HPC facilities and ecosystems.

The current document D6.1 describes structure and details of the training and education strategy and the plans of the events that will take place during the TREX project lifetime. The details included are the best available at the time of writing (regular updates are envisaged in due course). In addition to the training/education event and audience types mentioned above, various criteria are used to sort most of the planned activities: distinction is made based on subject (HPC, quantum chemistry), or between the planned and additional events, or between events internal to the consortium and events open to an external audience. The document D6.1 thus contains description of the overall strategy (Chapter 2) together with an overview and timeline for the planned events, internal training and education activities (Chapter 3), and, activities open to external audiences (Chapter 4). The events with an external outreach are each summarised on a summary-sheet that includes the currently available details (place, format, content, requirements, objectives, etc.). The early events are generally more detailed than the later ones. Promotion of training activities and engagement (Chapter 5) is followed by the Summary and perspectives (Chapter 6).

2 Overview of Training and Education Plan

In Section 2.1, the targeted audience is introduced. The planned outcomes of the TREX training and education program are described in Section 2.2. Section 2.3 presents general Training and Education strategy that is a key part of this document. A general overview of the planned events and actions is provided in Section 2.4. For definitions of some of the terms used, see Appendix A.

2.1 Groups targeted in TREX training activities

A brief overview of the training audiences is given in Table 1. Ensuring targeted training to TREX audiences is one of the objectives of the dissemination and communication strategy of the project. Among the stakeholders identified, the following groups will be involved in specific training activities:

I. End users in the educational and academic system. In particular:

   a. **Undergraduate and PhD students, postdocs, and researchers** (internal and external to TREX) in chemistry, materials science, and, more generally, in computational-oriented disciplines at universities, research centres, supercomputer centres, and experimental laboratories.
   TREX training aims here to increase the general literacy in quantum simulations and high-performance computing, boost the adoption of TREX codes, and also form a larger pool of developers via their engagement in TREX co-design activities.
   b. **Train the trainers.** TREX partners will promote "train-the-trainers" activities to improve the capacity building at their and other institutions, and impact the educational programs for (academic and non-academic) users in quantum chemical simulations and HPC applications.

II. Current and upcoming players in the European HPC ecosystem (external to TREX). TREX training is designed to enlarge the uptake of domain-specific and HPC applications in Europe. Several of its activities specifically aim at training a new generation of Computational Science researchers. This effort will be extremely beneficial, in particular, in member countries currently developing their HPC know-how and/or infrastructures. TREX training therefore closely aligns with the EuroHPC strategy and is expected to lead to a higher usage of HPC resources. Such a usage will be facilitated by the public availability of training instruments (webinars, lectures, videos) accessible together with TREX software via a single portal (developed within WP7) and of extended technical and co-design documentation. Furthermore, the setup of high-level technical support will assist the users of the TREX software platform in an optimized exploitation of current and future HPC infrastructures. In this endeavour, TREX will seek coordination with other CoEs, NCCs, and organizations (e.g., PRACE) on HPC and exascale computing so as to ensure cross-fertilization with the user community already engaged in currently funded CoEs. This coordination effort will induce larger resonance for TREX training activities, and avoid duplications. To this aim, TREX is already engaged in the activities of FocusCoE, participates to the CoE Council, and has active contacts with other CoEs and NCCs (in particular, MaX and MARVEL). Some hands-on workshops and schools for users and developers will be jointly organised.

III. 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. All of the training material developed within TREX will be made widely available to increase TREX scientific reputation and also to start scientific collaboration.

IV. 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 computer manufacturers. This may constitute the basis for collaboration related to hardware and/or software improvements (compiler/OS). In particular, benchmarking performance analysis of our HPC software for efficiency, scalability, energy efficiency, and numerical precision will be provided, and training will be organised on specific use cases of relevance to these target stakeholders. More generally, researchers in industry (e.g., manufacturing) will benefit from the activities listed under (I.a) and enhanced transfer of skills to industry will be attained via their attendance to the dedicated training sessions mentioned above (I.b). Training for industrial players will mainly consist of platform and co-design documentation, hands-on workshops or specific, industrial sessions as part of other end users' events.

While it would be perhaps too ambitious to consider policy stakeholders, funding agencies, and national authorities as target stakeholders for TREX training activities, they will be invited to some selected events. In particular, to 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 the Digital Europe Programmes. The Blueprint will be based on consultations resulting from TREX interactions with architects and integrators at HPC centers 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 raise awareness on the progress of TREX towards policy stakeholders.

Table 1: Overview of training audience and link to TREX.

	Type	Details and sample of stakeholders
I. End users in the educational and academic system	Code users	Researchers in academia
	Code developers	Field-specific and computer scientists Experts from HPC Centers
	Students	Undergraduate and PhD university students
	Postdocs	Postdocs at universities and HPC centers
	Researchers	Fields include: chemistry, materials science, atomic and molecular physics, condensed matter physics, computer science
	Educators	Scientists and officials related to education and curriculum development
II. Players in the European HPC ecosystem	Chemistry/physics/materials science CoEs and NCCs	Max, Nomad, MARVEL
	HPC CoEs and NCCs	PRACE, FocusCoE, PoP2, EuroCC/NSCC
	EU and national authorities	From national contact points to policy makers
III. Players beyond the European HPC ecosystem	Non-EU organizations, universities, CoEs, etc.	US Department of Energy, US Office of Basic Energy Sciences
IV. Hardware manufacturers and industrial players	Hardware industry	R&D departments focusing on HPC systems
	Code users in industry	Materials science researchers in industry

2.2   Outcomes

The general expected outcomes (results and consequences) of the planned training and education TREX events and actions (within WP6), within the whole project duration, are briefly summarized in Table 2.

Table 2: Overview of the expected outcomes of the TREX training and education program.

Type	Explanation
TREX code users uptake	Increased number of TREX users via events (schools, workshops, satellite events, hands-on sessions); envisaged are at least 50 end-users exploiting TREX codes in academia and industry; at least 10 occasions where TREX software is used as teaching tools.
TREX code developers uptake	Increased number of developers via TREX events (workshops, hands-on sessions, hackathons).
Increased literacy in HPC and awareness in high-accuracy quantum simulations and codes	Broad outreach to user communities also in countries advancing their HPC ecosystem; QMC as an accurate quantum method ready for exascale will receive more attention via training and education (communication and dissemination channels for creating awareness are addressed in WP7).
Higher and effective use of current and upcoming HPC infrastructures	TREX training and education program (events and technical support actions) will enlarge the pool of experienced users and developers of stochastic quantum software ready for future-generation of HPC infrastructures, thus promoting their sensible and efficient usage.

2.3 Training and Education Strategy

TREX training and education strategy is mainly intended for practitioners as well as HPC developers in materials science simulations, but has also a strong educational component. Goals of our strategy for internal and external training aim to:

- Provide introductory training in domain-specific and HPC fields:
  - Introduction to domain-specific background (high-accuracy quantum chemistry, QMC, HPC, etc.), basic concepts and techniques in programming and materials science.
- Provide advanced training:
  - Broaden the background knowledge, deepen conceptual and technical understanding, and extend the coverage of relevant topics at a higher level.
- Provide mentoring and hands-on experience (on-site, via events, via online consultation):
  - Mentor people on the newly obtained knowledge through experience (hands-on training to demonstrate the new techniques in practice).
  - Offer high-level technical support on use of software tools.
  - Ensure regular internal training and communication (e.g., via bi-weekly or monthly meetings for each WP).
- Provide education:
  - Incorporate the obtained knowledge and best training/education practices within existing or new curricula at universities.
  - Develop dedicated educational software and lecturing material.
  - Encourage TREX members to define a Personal Career Development Plan.

These goals will be achieved via the training/education activities of TREX, which consist of several hands-on workshops for code users and developers, hackathons, and a final school. These events will create new opportunities to facilitate the sharing of ideas among communities in different computational disciplines in molecular and materials science. Importantly, TREX events will not only focus on the domain-specific software of TREX but also on how it is integrated on (pre)exascale architectures with the most advanced developments, for example machine learning and data analytics. The consortium partners will be involved in lecturing and a key educational role will be played by the researchers at the HPC centers and the computer science UVSQ group to ensure the uptake of knowledge in their field. To engage a wide computational community and maximise the number of trained scientists/engineers, some of the TREX training activities will be held in collaboration with institutions that traditionally host events in the field of molecular and materials science (ICTP, CECAM, and Psi-k). Support to the code users and developers and development of education-purpose software are planned as well.

The general training and education plan is designed based on a systematic step-by-step building principle. For instance, HPC events (e.g., hackathons) will focus on distinct topics organized as a learning curve: programming, performance, scalability, and demonstrations. Similarly, the events for code users will mostly cover the following topics within each event: introduction to electronic structure and QMC topics, specific TREX QMC code(s) hands-on training, usage of AiiDA workflows and/or machine learning techniques with TREX code(s), and demonstrations.

Note that, below, where possible, differentiation is made between events for internal TREX members and events open to external audiences. Chapter 3 provides details regarding the internal activities and how will be ensured that the skills and knowledge of the members within the consortium are

sufficient to accomplish the ambitious goals of the project. The training and education plan for the events open to an external audience (in addition to the internal one) is addressed in Chapter 4.

Training at the time of COVID-19

Our original plans for training and education were relying on "classical" F2F meetings. Covid 19 advent has, however, forced us to fully reorganize our training and education activities. At the current stage, it seems that the training activities will take place online at least until the September 2021. One upside to the restrictions imposed by Covid 19 is that many TREX members who also have teaching duties at Universities had to master new technologies for performing lectures and exercise sessions online. Training and education activities within TREX, which will be fully online until summer 2021, will build on that expertise. It is expected that after the summer 2021, F2F training will be resumed in a complementary manner to online activities, hoping to get the best of both worlds. As an outcome of this online activity, the QMC and HPC events will be recorded and a full collection of those videos will be made available on popular channels such as Youtube.

TREX Training and Education Core Team

Table 3 provides a list of the core group of TREX consortium members actively involved in WP6 dedicated to Training and User uptake.

Table 3: Contact details of training and education responsible TREX members, and their contact-related expertise.

Who	Contact point for expertise
Matus Dubecky	WP6 coordinator Contact point with FocusCoE for training; Task leader: Domain-specific and HPC training via education (T6.3); training for code users in academia and industry (T6.2).
Cedric Valensi	Contact points with FocusCoE for training; Expert in online training
Fabio Affinito	Task leader: Technical Support for use of TREX Codes (T6.1); nucleating a new generation of code developers (T6.4).
Saverio Moroni	Task leader: Training for code users in academia and industry (T6.2).
Anthony Scemama	Task leader: Domain-specific and HPC training via education (T6.3).
Sandro Sorella	Task leader: Nucleating a new generation of code developers (T6.4).
William Jalby	Academic Training
Andrea Schillaci	Dissemination and outreach for training

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2.4   Schedule

The planned events open to external audiences and the training actions are summarized in Table 4. Figure 1 shows an indicative timeline.

Some of the events will be combined with other ones (organized outside TREX; e.g., satellite TREX events at conferences/symposia) in order to exploit synergy effect and achieve the largest possible outreach.

Table 4: Overview of the planned events (M-month, Q – year quartile, tbd – to be defined)

Event ID	Event/Action Type	Expected period	Linked to Task
ID001	Support Triage	M5-M36	T6.1
ID002	QMC Hands-on Workshop (STUBA)	2022 Q1	T6.2
ID003	Workshop (TUL)	2022 Q4	T6.2
ID004	Satellite Hands-on QMC tutorial	2022 Q3	T6.2
ID005	Final School	M36	T6.2
ID006	Winter School	2021 Q1	T6.3
ID007	Winter School	2022 Q1	T6.3
ID008	Winter School	2023 Q1	T6.3
ID009	Python Visual QMC application	M5-M36	T6.3
ID010	HPC Workshop (STUBA)	2023-Q1	T6.4
ID011	HPC Workshop (CECAM)	2022-Q4	T6.4
ID012	Hackathon I.	2021-Q2	T6.4
ID013	Hackathon II.	2021-Q4	T6.4
ID014	Hackathon III.	2022-Q1	T6.4
ID015	Hackathon IV.	2023-Q1	T6.4
ID016	Webinar	tbd	T7.1
ID017	Webinar	tbd	T7.1
ID018	Webinar	tbd	T7.1
ID019	Final Event	M34	T7.4

Figure 1: Indicative timeline with the overview of all events in TREX showing their purposed timing.
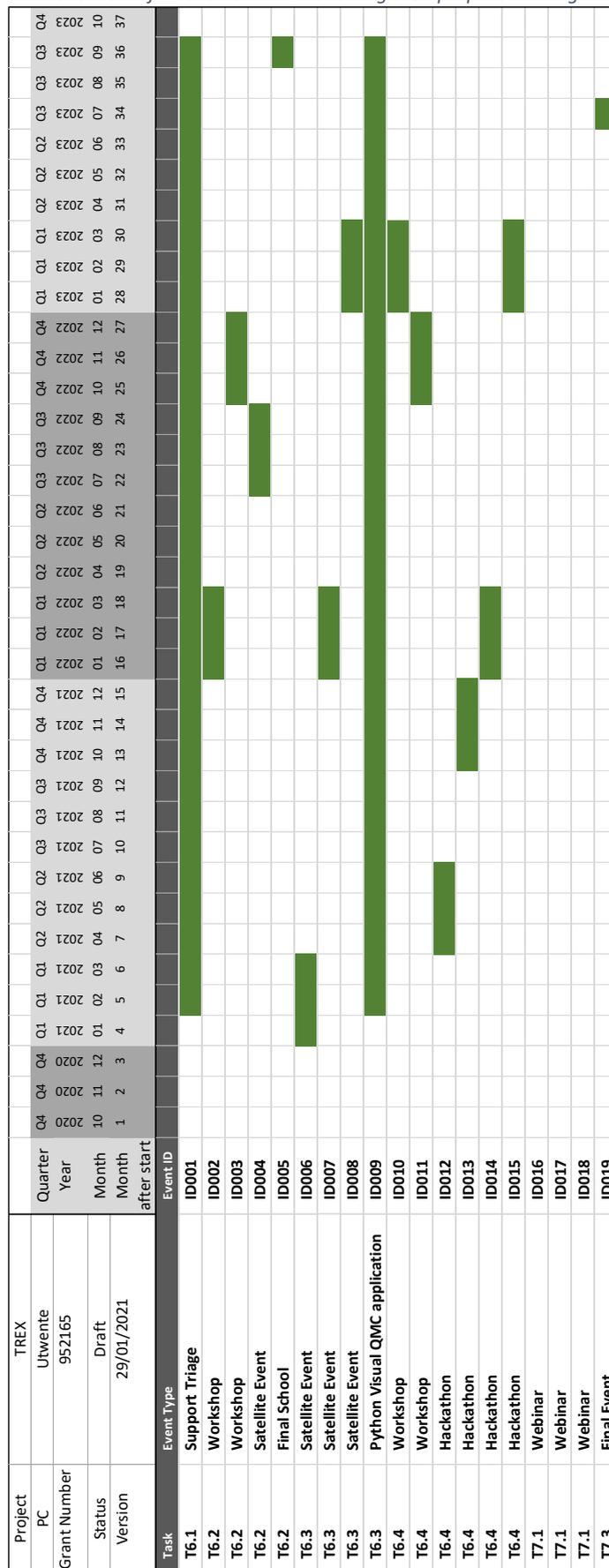
3 Internal Training and Education Activities

The goal of the internal training and education activities is to ensure that all members of the consortium are able to improve their individual levels of expertise. This is achieved by various types of training. In section 3.1, kick-off meetings, that contributed to the internal assessment of training needs of TREX members, and their objectives, are described in detail. The career development strategy of partners is summarised in section 3.2. The Collaboration of the researchers and juniors is elaborated in section 3.3. Implementation within the university educational programme is described in section 3.4. A good example of providing specific introductory training is shown in section 3.5 where the TREX partner, UVSQ, initiates education and training regarding the code performance evaluation.

3.1 Internal Assessment of Training Needs: WP Kick-Off Meetings

A series of kick-off meetings that took place during the TREX initial stage (Table 6) contained a large education component. The presented introductory lectures were intended so that the members of the TREX team are aware of the global picture and their responsibilities within the project. For instance, HPC experts had a chance to understand basic physics behind QMC methods, whereas QMC developers and practitioners had a chance to understand the code performance optimization basics. At the same time, the meetings provided an opportunity for internal assessment of training needs within the consortium. For instance, this led to demand for some specific (originally unplanned) training events (e.g., basics of code maintenance, github usage, etc., now planned with the help of the CodeRefinery project, see section 3.5.4 and Appendix B). Questions were raised frequently and answered by the presenters to the satisfaction of the attendees. Together with the attendee positive feedback, this confirmed that the kick-off-meeting presentations were generally useful and served their purpose.

Table 5: Kick-Off Meeting Overview

Date	Type of Meeting	Topic
06-10-2020	Kick-Off Meeting	General and managerial information
07-10-2020	Kick-Off Meeting	Chemists/physicists present field-specific content to computer scientists.
08-10-2020	Kick-Off Meeting	Computer scientists present field-specific content to chemists/physicists.
27-10-2020	Kick-Off Meeting – WP3	Engineering solutions for Exascale
28-10-2020	Kick-Off Meeting – WP1	Standard API for QMC kernels and implementation
02-11-2020	Kick-Off Meeting – WP2	Code modularization and interfacing Including education and training of the high-performance data analytics (HPDA) platform AiiDA
10-11-2020	Kick-Off Meeting – WP7	Communication, Dissemination and Engagement
03-12-2020	Kick-Off Meeting – WP6	Training, education, and users uptake
20-01-2021	Kick-Off Meeting – WP5	Demonstrations
To be defined	Kick-Off Meeting – WP4	Workflows for HTC and HPDA solutions, algorithms and toolkits

3.2   Personal Career Development Plan

Most institutions of the TREX consortium have in place a program to encourage and support their employees to continuously develop their personal and professional careers, most often in accordance with their institutional rules for career development.

Table 6: Individual Career and Development pages per partner provides links to the TREX consortium partners' websites with an explanation of career development plans (where available).

Table 6: Individual Career and Development pages per partner

Partner	Link to Career Development Plan
UT	https://www.utwente.nl/en/organisation/careers/career/career-development/
CNRS	https://carrieres.cnrs.fr/en/training-throughout-your-career
SISSA	https://www.sissa.it/
CINECA	https://pica.cineca.it/cineca/
FZJ	https://www.fz-juelich.de/careercenter/EN/Home/home_node.html
MPG	-
UVSQ	-
Megware	Internal Process with process ID M_PB_04 (accessible for all MEGWARE employees)
STUBA	https://www.stuba.sk/
UNIVIE	-
TUL	https://www.p.lodz.pl/en/hrlogo
TRUST-IT	-

3.3   Mentoring and Hosting Researchers

All TREX partners are well-established researchers who lead independent groups and have successfully supervised many junior scientists. They also have extensive experience in teaching and training, and have participated in, as well as organized, numerous advanced courses and schools in the fields of quantum chemistry and materials science, stochastic quantum simulations, and computer science. The junior TREX scientists (postdoc and software engineers) will join the host groups and institutions, and benefit from the additional local training and supervision expertise.

Furthermore, the junior scientists will also benefit from the interconnectivity between the consortium groups. The training at TREX events and at the host institutions will be supplemented by periods spent in the laboratories of the other partners. Such exchanges are an essential element of the overall internal training program, allowing TREX researchers to acquire new skills and special expertise unavailable at their home institution.

The mentoring effort by TREX partners will also reach researchers outside the consortium. The masters and PhD students, and postdocs of the TREX partners' groups will be encouraged to join some of the (internal and external) training events and will naturally access the knowledge and tools developed within TREX. Furthermore, individual laboratories of TREX routinely host researchers for collaborations involving TREX codes (for users and developers) and will keep doing so. The HPC-Europa3 program offers great opportunities to financially support such one-to-one exchanges also for extended periods.

3.4 University education

University education is the most effective way to guarantee that the new generation of students acquires the needed mindset to become active players in the upcoming radical HPC transformations. Within the duration of TREX project, valuable lessons will be learned and it is expected that these will propagate to the university curricula of the TREX academia partners. At the current stage, it is clear that these will mostly affect chemistry and HPC programmes (examples follow). Nevertheless, similar updates in other related fields, like, e.g., condensed matter physics, materials science, and beyond, are envisaged as well.

For curricula in chemistry, special courses targeting computational chemistry will likely be developed. These should go beyond just mathematical and numerical modelling and should cover topics ranging from how to master modern software development techniques to how to efficiently use large-scale computers. This will allow students in chemistry to fully use the power of numerical simulation which has become the third pillar of science together with theory and experiments. Many of these courses could be easily adapted to curricula in computational physics, biology, or materials Science.

Second, for curricula specialized in HPC (such as the 2 years UP Saclay/UVSQ Master program), TREX will allow to develop a set of courses illustrating the different key steps in computational science: starting from a theoretical model all the way down to a code able to perform useful computations. In a way, TREX is a unique project, because several different approaches will be used to solve basically the same problem. It will be particularly enlightening to analyze the pros and cons of each method involved.

3.5 Specific Training and Education Activities

This section provides an overview of the currently defined specific training and education activities identified as important during the kick-off meetings. These will likely be augmented by additional ones within the duration of the project lifetime.

3.5.1 Performance evaluation training for code developers

At the beginning of the TREX project lifetime, the internal TREX code developers will be trained regarding code performance evaluations. The TREX partner, UVSQ, will set-up a hands-on training for the code developers during workshops dedicated to each partner and their specific code. The format is a one-day or 2-day training course with general introduction and examples with a finalising session of performance evaluations on the actual codes. These events will take place in December 2020 or January 2021 using an online platform and the 6 (quantum chemistry) codes of the 5 TREX partners, see Table 7.

Table 7: TREX Codes and contact points

Code	Contact Person
Quantum Package	Anthony Scemama
QMC=Chem	Anthony Scemama
CHAMP	Claudia Filippi
TurboRVB	Sandro Sorella
GammCor	Kasia Pernal
NECI	Ali Alavi

At the current stage, the consortium already started with analysing and understanding the key applications of each involved partner and also provides them with one or two days of training on performance evaluation methods and tools. The training session will first consist of an introduction to the subject.   Hands-on sessions will follow subsequently. The results obtained from the performance tools applied to the partner applications will be presented along with a practical demonstration of how to use these tools and in particular how to deal with the diagnostics they provide.

A server (which will be protected and provide secure connections) will be set-up to let each application partner upload a representative/realistic version of their code including a few data sets. Having a server shared between the application developers and UVSQ will be extremely helpful to debug and to perform demonstrations.

3.5.2   Internal Training on Dissemination aspects by Trust-IT

To address the communication and dissemination needs of such a heterogeneous consortium like TREX, Trust-IT will organise dedicated internal training sessions. The purpose of such meetings is to align everybody's activity on different communication and dissemination aspects, including:

1. Types of content to be produced and shared and their relevance for the project; this includes, for instance, training on how to best exploit and contribute to the TREX website;
2. Channels, platforms and tools for the dissemination to be exploited by the project as well as by individuals; this includes, for instance, training on how to use social media channels in the context of the project;
3. Best practices for stakeholder engagement; this includes, for instance, training on content marketing techniques.

Leveraging on the acquired knowledge and skills will facilitate dissemination of the project results as a shared activity among all the consortium partners. These training moments will be organised in the framework of WP7 and offered on a voluntary basis to all partners.

3.5.3   VI-HPS Tuning Workshops

The VI-HPS (Virtual Institute – High Productivity Supercomputing) consortium aims at improving the quality and accelerating the development process of parallel applications using tools for HPC allowing to assist domain scientists in diagnosing programming errors and optimizing the performance of their applications. It regularly organises workshops to spread the use of these tools. During these workshops, participants are presented with a variety of performance tools and are given an opportunity of using them on their own codes with assistance from the tool developers.

One of these workshops took place in early December 2020. Although the scope of these workshops does not entirely cover the goal of the TREX training sessions described in section 3.5.1, participating to one of them could allow one to get a first overview of the main principles behind performance engineering and of the tools involved.

3.5.4   Introductory training on code development and code management

During the kick-off events (section 3.1), it was identified that some of the members of the project have a good experience in programming, but lack experience in modern tools used in collaborative code development (Git/GitHub, code review, continuous integration, ReadTheDocs, etc). The CodeRefinery infrastructure, supported by the Nordic e-Infrastructure Collaboration, provides periodically online training addressing this particular topic. Small groups of TREX members will register as a Team with an additional member of the team with more expertise identified as a helper. This procedure will be repeated during the project as long as the members need it (see Appendix B for the event details).

In addition, a training session will be organized for tools used specifically within TREX. Within WP1 it has been proposed to use org-mode notebooks to write the human-readable QMCkl implementation, to maintain consistency between the code and the related documentation. Hands-on sessions will be organised to enhance the productivity of the team. A second important topic is to address the differences between developing a code and a library (API design, constraints, dependencies) and specific technical aspects (compiling, linking and packaging). Finally, a large amount of our software will be integrated in the AiiDa framework. Hands-on sessions will also be required for the partners to integrate the use of AiiDa in they own workflows. The plan is to organize this training in April 2021, when most of the engineers and post-docs have already started working on the project.

4 External Training and Education

Multiple training and education events open to external audience are envisaged to take place during the TREX project lifetime. These events and actions will mostly focus on:

- how to create awareness on the TREX assets;
- how to foster the use of the developed codes;
- how to involve future-generation of HPC ecosystems.

As sketched above (section 2.2), a differentiation is made between events organised by the consortium for itself, and events organised by the TREX partners for external audiences (see event details below presented for each individual event, respectively). The sections below are divided between the planned events (section 4.1) and additional events that link to TREX (section 4.2).

4.1 Planned Events

For each of the planned events, all details available at the time of writing of this document are provided. Additional details will be provided in due time via updates of this document. The "tbd" shorthand used in the form sheets stands for the information that is unavailable at present, and needs "to be discussed" or settled later on. An overall risk assessment has taken place and is summarised in Appendix C: .

4.1.1 ID001 - Support Triage

TREX will offer the 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 requests for assistance will be conveyed.

The messages received from this mailbox will be classified according to their required level of assistance and the kind of help needed.

This support triage will be operated by an Operator-On-Duty (OOD), and the "trouble ticket" will be assigned to an expert (who could be a code expert or a person working in one of the computing centers). The expert will follow the evolution of the problem until the solution. All the steps will be tracked and documented.

Once the code is released and more scientists are added to the user base, a public mailing list might be implemented to allow a peer-to-peer troubleshooting mechanism. The support triage will still be in place for institutional users, such as new HPC facilities.

In case of TREX, this will be at the highest level on domain-specific and software issues. The technical support triage is meant to complement the support given by the computing centres and other HPC stakeholders (e.g., other CoEs such as MaX and PoP2, PRACE). This aims at solving contingent software problems, as well as offering the users help in finding the best strategy to address their specific problems [2].

Task Scope	
Work Package	WP6 Training and user uptake
Task	T6.1
Task Title	Technical support for the use of TREX codes
Task Responsible	Lead: F. Affinito - CINECA
Event Objectives	Description
Users support	Deliver technical and scientific support to the users in a timely manner to troubleshoot and facilitate adoption of the code.
Event Target Audience	Description of audience and expected number of participants, entry level
Code users	Scientists who want to apply the TREX code/s to systems that present challenge, or face technical problems with code inputs.
HPC Users	Users with problems in using the code/s on HPC clusters.
Pre-Requirements	Detail what is required before
Infrastructure	Single Point of Contact, i.e., webpage or mailbox.
Support Team	List of operators in charge of assigning tickets to experts.
Experts List	List of available domain experts.
Impact after event	Detail what impact is targeted
Exploitation of HPC	Maximise the usage of HPC facilities.
Improvement of the production level	Enhance the productivity of researchers by providing timely support.

4.1.2 ID002 – QMC Hands-on Workshop (STUBA)

Event Overview			
Event ID	ID002	Event Linked	ID010
Event Title	QMC Hands-on Workshop	Event Period	2022-Q1
Event Type	Workshop	Event Date	3 days
Event Location	Slovakia	Event Country	Slovakia
Event Coordinator	Matus Dubecky	Event Organisation	STUBA
Event Description	ID002-T6.2 Workshop STUBA Slovakia		

Event Scope	
Work Package	WP6 Training and user uptake
Task	T6.2
Task Title	Training for code users in academia and industry
Task Responsible	Lead: M. Dubecky - STUBA; S. Moroni - SISSA
Event Objectives	Description
Basic QMC training	Crash-course in practical electronic structure QMC theory and computations (8 hours).
Basic TREX code/s hands-on training	Practical entry-level QMC hands-on sessions using TREX codes (VMC, DMC, molecules, solids) in the domain of molecular and materials science. (4x2hours).
Special topics	ML tools (4 hours) and the workflow structure integrated in AiiDA (4 hours).
Event Target Audience	Description of audience and expected number of participants, entry level
Code users	Audience: (preferentially local) MSc. and PhD Students, postdocs, researchers Entry level: electronic structure-interested students/researchers with proven experience in DFT, quantum/physical chemistry, computational materials science, condensed matter or computational physics, etc. No. of participants: 20
Pre-Requirements	Detail what is required before
codes ready for use	The universal TREX I/O library should be operable with TREX codes and debugged for the tasks described in event objectives.
Impact after event	Detail what impact is targeted
Increased QMC awareness	Most of the expected participants will not have any experience with QMC. Their participation will likely increase the number of members of the "QMC-aware" community.
New QMC users	An increased number of QMC users is expected due to the participation of the target audience, that have not been using QMC in their research before.
More TREX code users	More inexperienced users will have chance to interact with TREX codes, participants already using QMC in their research will have chance to find better solutions for their research.

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.

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4.1.3 ID003 – Workshop (TUL)

Event Overview			
Event ID	ID003	Event Linked	-
Event Title	tbd	Event Period	2022-Q4
Event Type	Workshop	Event Date	Tbd
Event Location	TUL	Event Country	Poland
Event Coordinator	Kasia Pernal	Event Organisation	TUL
Event Description	ID003-T6.2 Workshop TUL Poland		

Event Scope	
Work Package	WP6 Training and user uptake
Task	T6.2
Task Title	Training for code users in academia and industry
Task Responsible	Lead: M. Dubecky - STUBA; S. Moroni – SISSA
Event Objectives	Description
Machine Learning	Focus on how to use the TREX platform together with the machine learning (ML) tools In the domain of molecular and materials science.
Workflows	Understanding and applications of the workflow structure integrated in AiiDA.
Event Target Audience	Description of audience and expected number of participants, entry level
Code users	PhD student and post-doc's mainly but also more senior code users. The expected number of participants: 50.
Pre-Requirements	Detail what is required before
Code interface	Interface allowing exchange of data between quantum chemistry TREX codes should be ready.
Preliminary knowledge	Basic knowledge of quantum chemistry methods, basic understanding and skills in running quantum chemistry calculations.
Impact after event	Detail what impact is targeted
More users of TREX codes	Participants will be able to use TREX quantum chemistry codes and their interfaces. They will learn about the capabilities of the codes.

4.1.4   ID004 – Satellite Hands-on QMC tutorial

Event Overview			
Event ID	ID004	Event Linked	CESTC 2022
Event Title	Hands-on QMC tutorial	Event Period	2022-Q3
Event Type	Satellite Event	Event Date	Sep 2022 (2 days, extending CESTC)
Event Location	Where the Central European Symposium on Theoretical Chemistry 2022 takes place (Slovakia or Hungary)	Event Country	Slovakia or Hungary
Event Coordinator	Matus Dubecky	Event Organisation	STUBA
Event Description	ID004-T6.2 Satellite Event CESTC Slovakia		

Event Scope	
Work Package	WP6 Training and user uptake
Task	T6.2
Task Title	Training for code users in academia and industry
Task Responsible	Lead: M. Dubecky - STUBA; S. Moroni – SISSA
Event Objectives	Description
Basic QMC introduction	Crash-course in practical electronic structure QMC theory and computations (8 hours)
Basic TREXC code/s hands-on training	Practical entry-level QMC hands-on sessions using TREX codes (single-determinant and multideterminant VMC & DMC, total energy computations in molecules & solids) in the domain of molecular and materials science (8 hours)
Event Target Audience	Description of audience and expected number of participants, entry level
Code users	Audience: MSc. and PhD. Students, postdocs, researchers Entry level: QMC-interested participants of CESTC (Central European Symposium on Theoretical Chemistry) 2022 participants No. of participants: 20
Pre-Requirements	Detail what is required before
TREX QMC suite of codes ready for use	The universal TREX I/O library should be operable with TREX codes and debugged for the tasks described in event objectives.
Impact after event	Detail what impact is targeted
Increased QMC awareness	Most of the expected participants do not have any experience with QMC. Their participation will likely increase the number of members of the "QMC-aware" community.
New QMC users	The number of QMC users will likely grow due to the participation of the target audience, that mostly have not been using QMC in their research.

4.1.5   ID005 Final school

Event Overview			
Event ID	ID005	Event Linked	-
Event Title	tbd	Event Period	Sept 2023
Event Type	Final School	Event Date	tbd
Event Location	ICTP or CECAM	Event Country	tbd
Event Coordinator	Claudia Filippi	Event Organisation	-
Event Description	ID005-T6.2 Final School ICTP or CECAM		

Event Scope	
Work Package	WP6 Training and user uptake
Task	T6.2
Task Title	Training for code users in academia and industry
Task Responsible	Lead: M. Dubecky - STUBA; S. Moroni - SISSA
Event Objectives	Description
Training in TREX software and methodology	The school will be in the domain of molecular and materials sciences, and will focus on how to use TREX software platform together with the ML tools and the workflow structure integrated in AiiDA. The school will alternate lectures covering the introductory concepts of the relevant methodologies with hands-on training sessions.
Event Target Audience	Description of audience and expected number of participants, entry level
Code users	50-100 participants. PhD students, postdocs, and researchers in academia and industry.
Pre-Requirements	Detail what is required before
General field-specific knowledge	Background in electronic structure theory
Impact after event	Detail what impact is targeted
Increased use of TREX HPC software.	Promote the use of TREX codes within academia and industry; significantly enlarge user community; foster use of HPC codes.

4.1.6   ID006 – ID007 – ID008 Winter school

Event Overview			
Event ID	ID006	Event Linked	-
Event Title	Tbd	Event Period	25 Jan - 5 Feb 2021
Event Type	Satellite Event	Event Date	4 Feb
Event Location	Luchon Winter School of the Erasmus Mundus Joint European Master Degree program in Theoretical Chemistry and Computational Modeling	Event Country	Online
Event Coordinator	Claudia Filippi, Anthony Scemama	Event Organisation	-
Event Description	ID006-T6.3 Satellite Event Luchon Winter School Erasmus Mundus		

Event Scope	
Work Package	WP6 Training and user uptake
Task	T6.3
Task Title	Domain-specific and HPC training via education
Task Responsible	Lead: A. Scemama - CNRS; M. Dubecky - STUBA
Event Objectives	Description
Basic QMC Training	The "Tutorials in Theoretical Chemistry" Luchon Winter School focuses on the computer implementation of methods in quantum chemistry. The tutorials include: Advanced programming techniques; Geometry and Topology: Building Nanoparticles; Low-dimensional Carbon structures: the usefulness of simple approaches; Quantum Magnetism: the Heisenberg model; Quantum Dynamics: Propagating wave packets; Vibrations in Molecules: Harmonic/Morse Oscillators. TREX will participate by teaching one extra day to introduce the basic concepts of QMC methods and explain how to write a simple QMC program.
Event Target Audience	Description of audience and expected number of participants, entry level
Students	Audience: master students and 1st-year PhD students Number of participants: 25-35 participants. Usually, the number of participants is higher since the event is also open to masters and 1st-year PhD students outside the Erasmus program. However, this year, the school will be online because of COVID and the organizers will limit the participation to the Erasmus Mundus Students due to the difficulties of organizing effective online hands-on sessions for a much larger audience.

Pre-Requirements	Detail what is required before
Background	Basic knowledge of programming. Basic knowledge in quantum chemistry.
Impact after event	Detail what impact is targeted
Increased number of students interested in electronic structure	Educating young students in quantum chemistry, programming, and QMC methods. Already during the master's degree, students will be able to appreciate the capabilities of these sophisticated stochastic approaches and consider them as a valuable tool for future applications.
Related Document	Description
Web page	https://www.irsamc.ups-tlse.fr/lttc/

Analogous events (ID007 and ID008) are envisaged to take place in two upcoming years (2022 and 2023), and will be open to extended audience of master students with respect to the 2021 event.

4.1.7 ID009 – Python visual QMC application

Task Overview			
Task ID	ID009	Event/task Linked	-
Task Title	PVQA	Task Period	M5-M30
Task Type	Python Visual QMC application	Task Description	ID009-T6.3 Python Visual
Task Coordinator	Matus Dubecky	Task Organisation	STUBA

Event Scope	
Work Package	WP6 Training and user uptake
Task	T6.3
Task Title	Domain-specific and HPC training via education
Task Responsible	Lead: A. Scemama - CNRS; M. Dubecky - STUBA
Event Objectives	Description
Development of Python-based visual QMC application for educational purposes	The goal is development of a black-box intuitive QMC Python-based application. Its main purpose is barrier-less demonstration of basic QMC ideas in a way open to unexperienced users (they can learn by trying various functionalities, trial and error, etc.) The basic topics will cover particle ensembles, histograms, ground-state projection techniques, simple DMC vs importance sampling DMC, fixed-node approximation, imaginary-time-dynamic mode, statistical analysis of the output data, 3D view with the on-the-fly plots, etc. The models will include simple 3D low-dimensional systems (hydrogen atom, helium atom, H2+ or so). The application will be accessible from the TREX website.
Event Target Audience	Description of audience and expected number of participants, entry level
Students, researchers, others	Audience: university students, researchers, and, any other audiences interested to "play" with the application in a black-box manner Entry level: N/A Participants: unlimited
Impact after event	Detail what impact is targeted
Boosting computational physics and QMC awareness	Code users will have chance to "play" with QMC method without barriers or a priori knowledge. This increases likelihood of their future interest in (computational) physics, QMC methods, etc.

4.1.8 ID010 – HPC Workshop (STUBA)

Event Overview			
Event ID	ID010	Event Linked	ID002
Event Title	TREX HPC Workshop	Event Period	2023-Q1
Event Type	Workshop	Event Date	tbd, 2-3 days
Event Location	Slovakia	Event Country	Slovakia
Event Coordinator	Matus Dubecky	Event Organisation	STUBA, EuroCC/NSCC
Event Description	ID010-T6.4 Workshop Slovakia		

Event Scope	
Work Package	WP6 Training and user uptake
Task	T6.4
Task Title	Nucleating a new generation of code developers
Task Responsible	Lead: S. Sorella - SISSA; F. Affinito - CINECA
Event Objectives	Description
Increasing HPC literacy	The attendee code developers will have chance to increase their HPC literacy with help of EuroNCC/NSCC competence centre (https://eurocc.nscc.sk)
Software development using QMCkl library	Training will cover how to implement new functionalities in the QMCkl libraries and how to integrate them into the external codes; focus on domain-specific software developments; how these are integrated on the upcoming (pre)exascale architectures.
Event Target Audience	Description of audience and expected number of participants, entry level
Code Developers	Code Developers will take advantage from this event learning computational techniques and programming models that will improve the quality of their codes, their performance and the optimal exploitation of the computational resources
Pre-Requirements	Detail what is required before
Programming	A good knowledge of C and/or Fortran and/or C++ is required in order to work on the codes. A knowledge of the MPI, OpenMP and CUDA is strongly suggested.
Impact after event	Detail what impact is targeted
Increased HPC literacy	Improvement of the programming skills and HPC literacy of the attendees.
New functionalities	Implementation of new functionalities in the QMCkl.
Optimal usage of CPU resources	Optimal exploitation of the computational resources (in particular, of the pre-exascale systems)

4.1.9   ID011 – HPC Workshop (CECAM)

Event Overview			
Event ID	ID011	Event Linked	-
Event Title	tbd	Event Period	2022-Q4
Event Type	Workshop	Event Date	tbd
Event Location	CECAM node	Event Country	tbd
Event Coordinator	Fabio Affinito	Event Organisation	CECAM
Event Description	ID011-T6.4 Workshop CECAM node		

Event Scope	
Work Package	WP6 Training and user uptake
Task	T6.4
Task Title	Nucleating a new generation of code developers
Task Responsible	Lead: S. Sorella - SISSA; F. Affinito - CINECA
Event Objectives	Description
Code development training	The objective of this event is the training of code developers in order to make them able to implement new functionalities in the QMCkl libraries and to integrate them into codes external to the consortium. Focus will be put on the domain-specific software developments, providing the attendees with techniques aimed to make the codes more performant on the EuroHPC (pre)exascale architectures. This will result on a better exploitation of the HPC infrastructures and, on the user side, improvement of the capability to solve more complex and challenging use cases.
Event Target Audience	Description of audience and expected number of participants, entry level
Code Developers	Code Developers will take advantage from this event by learning computational techniques and programming models that will improve the quality of their codes, their performance and the optimal exploitation of the computational resources
Code users	Code users interested in code development will learn how to modify the codes in order to implement their models, enriching the functionalities of QMCkl and widening the spectrum of the use cases.
Pre-Requirements	Detail what is required before
Programming languages	A good knowledge of C and/or Fortran and/or C++ is required in order to work on the codes. A knowledge of MPI, OpenMP and CUDA is strongly suggested.
Impact after event	Detail what impact is targeted
Improved skills	Improvement of the programming skills of the attendees.
Improved functionality	Implementation of new functionalities in the QMCkl.
Optimal use of resources	Optimal exploitation of computational resources (in particular, of the pre-exascale systems)

4.1.10 ID012 Hackathon I.

Event Overview			
Event ID	ID012	Event Linked	-
Event Title	TREX Hackathon I.	Event Period	2021-Q2
Event Type	Hackathon	Event Date	tbd
Event Location	tbd	Event Country	tbd
Event Coordinator	A. Scemama	Event Organisation	tbd
Event Description	ID012-T6.4 Hackathon		

Event Scope	
Work Package	WP6 Training and user uptake
Task	T6.4
Task Title	Nucleating a new generation of code developers
Task Responsible	Lead: S. Sorella - SISSA; F. Affinito - CINECA
Event Objectives	Description
Design principles for a library	What is an API? Portability Dangers of mutability Type safety Error handling
Org-mode	Literate programming Reproducible research
Programming with IRP	What is IRP programming Hands-on session
AiiDA	Hands-on session
Event Target Audience	Description of audience and expected number of participants, entry level
Code owners, new developers, university students	Maximum 30 participants, priority given to TREX members
Pre-Requirements	Detail what is required before
TREX members	None
University students	Linux OS, programming in a compiled language
Impact after event	Detail what impact is targeted
Increased attendee proficiency	All TREX developers will become proficient with the common tools
Understanding the library development procedure	All TREX developers understand the software particularities in developing a library

4.1.11 ID013 – Hackathon II.

Event Overview			
Event ID	ID013	Event Linked	-
Event Title	TREX hackathon II.	Event Period	2021-Q4
Event Type	Hackathon	Event Date	tbd
Event Location	tbd	Event Country	-
Event Coordinator	W. Jalby	Event Organisation	UVSQ
Event Description	ID013-T6.4 Hackathon		

Event Scope	
Work Package	WP6 Training and user uptake
Task	T6.4
Task Title	Nucleating a new generation of code developers
Task Responsible	Lead: S. Sorella - SISSA; F. Affinito - CINECA
Event Objectives	Description
Performance evaluation at the next level	Learn how to use analysis tools to improve the performance and optimise the numerical accuracy of the codes. Use these methods to achieve improvements on the participants' own codes.
Event Target Audience	Description of audience and expected number of participants, entry level
Code developers	This targets developers who wants to improve their codes and learn methods to do this. The expected number of different codes should be around 3 to 4, with 2 to 3 developers per code.
Pre-Requirements	Detail what is required before
Machine ready before event	Local servers accessible to consortium Codes to optimise installed on the servers Possibility to install tools before the event Some notions of the basics of performance optimisation - Vectorisation - Memory hierarchy - Scalability - Numerical accuracy
Impact after event	Detail what impact is targeted
Code improvements	Improvements to the codes involved
Performance optimization skills	Better awareness of the pitfalls of performance optimisation

4.1.12 ID014 – Hackathon III.

Event Overview			
Event ID	ID014	Event Linked	-
Event Title	TREX hackathon III.	Event Period	2022-Q1
Event Type	Hackathon	Event Date	tbd
Event Location	-	Event Country	-
Event Coordinator	F. Affinito, W. Jalby	Event Organisation	CINECA / UVSQ
Event Description	ID014-T6.4 Hackathon		

Event Scope	
Work Package	WP6 Training and user uptake
Task	T6.4
Task Title	Nucleating a new generation of code developers
Task Responsible	Lead: S. Sorella - SISSA; F. Affinito - CINECA
Event Objectives	Description
Tuning QMCkl and QMC codes	The attendees will learn how to tune the execution parameters and how to modify the codes in order to achieve the highest scalability on the Leonardo pre-exascale machine.
Workflow optimization	The attendees will learn how to deploy complex workflows with QMC codes in the Leonardo supercomputer.
Learning how to use Leonardo supercomputer	The attendees will learn the features of the Leonardo supercomputer and how to run at best on it.
Event Target Audience	Description of audience and expected number of participants, entry level
Code owners, experienced users, and technologists	The hackathon will involve code users, code developers and HPC technologists. By collaborating they will achieve the tuning of the QMC flagship codes and the best implementation of QMCkl in order to exploit at the best the capabilities of the Leonardo machine.
Pre-Requirements	Detail what is required before
Code knowledge	All the participants are supposed to have a good knowledge of the QMC flagship codes of TREX and be familiar with the fundamentals of parallel computing.
Workloads/workflows	Availability of workloads and workflows to use in order to tune the performances of the codes
Impact after event	Detail what impact is targeted
Exploitation of HPC resources	This event will permit to improve the scalability of QMCkl and the QMC codes and to test the features of the Leonardo machines with these workloads.
Success story	This will prepare the possibility to run challenging calculations on one of the most powerful machines in Europe at the time of the event.

4.1.13 ID015 – Hackathon IV.

Event Overview			
Event ID	ID015	Event Linked	-
Event Title	TREX Hackathon IV.	Event Period	2023-Q1
Event Type	Hackathon	Event Date	6-10.2.2023 or 20-24.2.2023
Event Location	Juelich Supercomputing Centre	Event Country	Germany
Event Coordinator	D. Pleiter	Event Organisation	FZJ
Event Description	ID015-T6.4 Hackathon		

Event Scope	
Work Package	WP6 Training and user uptake
Task	T6.4
Task Title	Nucleating a new generation of code developers
Task Responsible	Lead: S. Sorella - SISSA; F. Affinito - CINECA
Event Objectives	Description
Demonstrate performance of TREX software on state-of-the-art HPC systems	This event takes place at a late stage of the project and will serve as a final opportunity to optimise codes.
Event Target Audience	Description of audience and expected number of participants, entry level
Code owners and developers	Up to 15 code owners and developers
HPC experts from HPC data centres and HPC technology providers (e.g., NVIDIA)	5 HPC experts
Pre-Requirements	Detail what is required before
Sufficient number of HPC experts	Sufficient number of HPC experts to support participating code owners and developers (aim for a 1:3 ratio)
Access to machines	Pre-installed online machines with secure connection ready for use during the event
Impact after event	Detail what impact is targeted
Increased efficiency	Publicly available software running efficiently on state-of-the-art HPC systems

4.1.14 ID016 - ID017 - ID018 – TREX Webinar series

Event Overview			
Event ID	ID016 - ID017 - ID018	Event Linked	-
Event Title	TREX Webinars on transfer of research results and service offers	Event Period	tbd
Event Type	Webinar	Event Date	tbd
Event Location	tbd	Event Country	tbd
Event Coordinator	Sara Pittonet (Trust-IT)	Event Organisation	Trust-IT
Event Description	ID016 - ID017 - ID018 Webinars		

Event Scope	
Work Package	WP7 Communication, Dissemination and Engagement
Task	T7.3
Task Title	TREX outreach strategy and synergies with related HPC initiatives
Task Responsible	Sara Pittonet (Trust-IT)
Event Objectives	Description
Engage users	The organisation of three webinars is part of the overall T7.1 in charge of producing general and targeted communication activities to raise awareness and engage end users, and relevant initiatives and collect their feedback.
Raise awareness	The TREX suite of inter-operable flagship codes and libraries. Opportunities for the industrial stakeholders. The scope and structure of each single webinar will be further defined during the project timeframe according to the project developments.
Event Target Audience	Description of audience and expected number of participants, entry level
Scientific users, developers, scientists	Academic end users in HPC and quantum simulations and members of the HPC ecosystem; Hardware manufacturers and industrial players
Pre-Requirements	Detail what is required before
TREX platform and components are released	The timeframe for the delivery of the webinars will be built following the first release of the software platform (M18) and its components
Impact after event	Detail what impact is targeted
Increased awareness and more users engaged	At least 30 stakeholders reached through the TREX webinars by M36.

4.1.15 ID019 Final Event

Event Overview			
Event ID	ID019	Event Linked	-
Event Title	TREX Final-Results-Oriented Event	Event Period	M34
Event Type	Final Event	Event Date	M34
Event Location	tbd	Event Country	tbd
Event Coordinator	Sara Pittonet	Event Organisation	Trust-IT
Event Description	ID019-T7.3 Final Event		

Event Scope	
Work Package	WP7 Communication, Dissemination and Engagement
Task	T7.3
Task Title	TREX outreach strategy and synergies with related HPC initiatives
Task Responsible	Sara Pittonet (Trust-IT)
Event Objectives	Description
Delivery of the main TREX results and launch of the TREX Blueprint	A TREX final event will be organised focussing on the dissemination of results and highlighting the relationships with other CoEs, as an opportunity to deliver the TREX BluePrint to the funding agencies and to policy makers and the stakeholders from TREX.
Event Target Audience	Description of audience and expected number of participants, entry level
Scientific users, developers, scientists; policymakers, funding agencies, national authorities	The final event will target all TREX stakeholders, as well as the Members of the European HPC ecosystems industry representatives to foster wider access, usage, and uptake of knowledge in HPC and in the development of a scalable eco-system of TREX codes within an integrated HPC, HTC, and HPDA framework. Policymakers, funding agencies, and national authorities will be invited to present them priorities, challenges, and gaps emerging from the TREX project that can be further addressed under Horizon Europe and the Digital Europe Programmes.
Pre-Requirements	Detail what is required before
Drafting of the TREX Blue print	TREX BluePrint for policy makers, to pave the way for main recommendations for future work programmes.
Impact after event	Detail what impact is targeted
Recommendations up taken by policy makers, funding agencies and national authorities	The event is expected to launch and leave as a legacy of the project a set of key recommendations targeting TREX scientific user communities, developers, and scientists in materials sciences to foster wider access, usage, and uptake of knowledge in HPC and in the development of a scalable eco-system of TREX codes within an integrated HPC, HTC, and HPDA framework. The Blueprint will also target policymakers, funding agencies, and national authorities to guide them on which priorities, challenges, and gaps can be further addressed under Horizon Europe and the Digital Europe Programmes.

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.

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4.2 Additional events

Besides the events defined in the Grant Agreement [2], the TREX partners will also be engaged in a number of additional events. To engage a wide computational community and maximise the number of trained scientists/engineers, some of the TREX training activities (hands-on workshops, schools) will be organized in collaboration with other CoEs (NOMAD, MaX, …), and institutions that traditionally host events in the field of molecular and materials science (ICTP, CECAM, and Psi-K).

A promising example of a school organized by the TREX consortium member (SISSA) and Psi-K community, is the TurboRVB School that will take place in Trieste (Italy) under TREX auspices from Jul 12 to Jul 23, 2021. The school schedule will be divided into lectures and hands-on sessions, given by the TurboRVB developers and other lecturers, from the TREX consortium. This event will be compliant with the TREX legacy of feeding a stronger community of QMC users and developers.

This event is focused on students without expertise in electronic structure theory and computations. Its aims may be summarized as:

- providing undergraduate students with a basic but detailed overview of the theoretical foundations of QMC computer simulations;
- giving an overview of the domains of interesting applications;
- providing the basics for writing and running practical simulations using TurboRVB, a TREX QMC code

5   Promotion of training activities and engagement

The TREX website will be the main entry point for all the training materials collected and made available for the project stakeholder as well as 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. Training materials including the recorded sessions of online training activities, will be published and made available to registered users, together with contributions to university courses and curricula, train-the-trainers materials, and train through research opportunities (internships and exchanges at TREX partner institutes, see section 3.3). Guidelines for industry stakeholders will also be part of the training area, together with the information and materials about TREX training workshops and events. Last but not least, the Docker container developed by the CNRS-Toulouse partner to allow the participants of the training to work in the same software environment will be accessible from this training area.

All necessary communication and outreach channels will be used to ensure the promotion of the training activities and engagement of target users. Target content will be produced and continuously updated, in liaison with WP6 team, 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 will be exploiting Twitter and LinkedIn, to build its community and to communicate all the training opportunities to a wide audience. Twitter will be mainly used for real-time updates and to promote workshops and webinars, while LinkedIn will be mainly used to advertise specific events (event pages on LinkedIn will be created on purpose), attract new stakeholders, send targeted messages, and create and follow discussion groups.

The details of the training programme promotion as well as the activities envisaged to attract training participants will be described in more detail as a part of the communication and dissemination plan (deliverable D7.3).

6 Summary and perspectives

In summary, the document D6.1 provides an overview of the general training and education strategy implementation within WP6 of the TREX consortium project. This covers audience types, overview of events with a timeline, and details of all events as known at the time of writing (regular updates are envisaged in due course).

Regarding the event planning, the follow-up work related to the training and education plan includes: date and programme settlement for each event, design of appropriate surveys as evaluation measures, decisions related to the possible financial support of participants and their selection process if the number of applicants exceeds the maximum number of seats, etc.

On the deliverables side, the following additional WP6 deliverables are scheduled to be provided within the project duration:

· Updates to the D6.1: *TREX Training and Education Strategy and Plan.*

· D6.2: *First report on the status of organisation of training events and activities, including validation surveys and educational QMC application* (M20).

· D6.3: *Final report on training, including validation surveys, the educational QMC application, training assessment recommendations, and lessons learned* (M36).

Last but not least, future work includes the organization of individual events and taking the related post-event measures (preparation of reports with validation surveys, summary, etc.).

7 References

[1] http://www.ambysoft.com/essays/trainingAndEducation.html

[2] Grant Agreement No. 952165

[3] https://ec.europa.eu/info/topics/education-and-training_en

Appendix A: Definition of terms

A.1 Definitions

The definitions presented in the current section enable the reader to properly interpret the meaning of some of the key terms used below.

Training

Training is the process by which people gain tangible skills that they can start applying immediately [1].

Education

Education is the process by which people gain knowledge and understanding [1].

Technical Support

Technical Support is the process by which people are assisted in order to solve specific problems. For more details. see section 4.1.1.

Python Visual QMC application

An educational-purpose Python-based visual and modular QMC application (to be shared via TREX website). For more details. see section 4.1.7.

Training type

A brief overview of the different types of trainings and explanation is given in Table 8. This is meant as guidance to clarify all events and actions.

Table 8: Training types and explanation

Type	Explanation
Workshop	Multiple workshops are planned in due course
Satellite Event	Satellite events are planned as a part or extension of other more general events. E.g., in order to outreach to the central-Europe theoretical chemistry audience, QMC tutorial will take place as a satellite event of CESTC symposium (section 4.1.4).
Final School	A final TREX school for code users, see section 4.1.5.
Hackathon	For a Hackathon a clear focus and defined objective need to be selected. This will be explored with multiple stakeholders (experts for their in-depth knowledge and non-experts to think from out-of-the-box perspective) at a specified amount of time to reach specific goal/s. For instance, a single hackathon event may have a specific goal like explicitly verified code performance improvement/s etc.
Webinar	Multiple webinars for internal as well as external audiences will take place (section 4.1.14)
Final Event	A final TREX event, see section 4.1.15

Appendix B: CodeRefinery Workshop

Event Overview			
Event ID	-	Event Linked	-
Event Title	CodeRefinery workshop	Event Period	2020
Event Type	Workshop	Event Date	Nov 17-19, 24-26, 9:00 - 12:00
Event Location	Online	Event Country	-
Event Coordinator	A.Scemama	Event Organisation	CodeRefinery
Event Description	T6.4 Code Refinery training		

Event Scope	
Work Package	WP6 Training and user uptake
Task	T6.4
Task Title	Nucleating a new generation of code developers
Task Responsible	Lead: S. Sorella - SISSA; F. Affinito - CINECA
Event Objectives	Description
	Become familiar with tools and best practices for version control and reproducibility in modern research software development. The main focus is on using Git for efficiently writing and maintaining research software.
Event Target Audience	Description of audience and expected number of participants, entry level
Code owners, new developers, post-docs	Code owners, new developers and TREX post-docs
Pre-Requirements	Detail what is required before
Linux literacy	Participants should be able to navigate the file tree in a terminal session and edit text files in the terminal. Basics in one or more programming languages. Have a basic idea of how Git works.
Required installed software	Bash; Editor; Git, including some configuration; (optional) Visual diff tools; Python; Jupyter and JupyterLab; (optional) Snakemake; Zoom
Impact after event	Detail what impact is targeted
Improved skills	Better use of Git/GitHub by all the participants
	Basic knowledge on FAIR data and reproducible research
	Improved quality of software documentation
	Basic knowledge on continuous integration and automated testing
Related Document	Description
Web page	https://coderefinery.github.io/2020-11-17-online/

Risk Management	
Risk Identified	Mitigation Strategy
Human interaction is missing	Online course with ~90 participants; risk of missing personal interactions of participants with the instructors. Anthony Scemama is a helper for the TREX Team, he will improve the interaction with participants.

Appendix C: Risk Management for events and actions

The organisation of the different events involves multiple risks. An overall risk management assessment has taken place. The risks identified and their mitigation strategy are summarised in Table 9. Each individual event will go through some more careful assessment of the risks by the organizing party.

Table 9: Risks Identified and their mitigation strategy

Risk Identified	Mitigation Strategy
Current Operator-On-Duty not assigning trouble tickets	A backup operator is in charge of the procedure.
No solution was provided by the designated expert in due time.	The ticket is automatically resubmitted to the SPC and then assigned to a different (scientific or HPC) expert.
It is difficult to assess if the students have a good understanding (during online events).	Use lessons learned from current online events such as breakout rooms with small numbers of people, an interactive online document to ask questions, etc.
Force majeure still prevents the organisation of physical meetings	The event will be organised as an online event leveraging on state-of-the art virtual events software, platforms and services.
CECAM will decide not to grant the event	The event will be financed with other resources (in-kind of partners, Psi-k, etc.)
Temporary unavailability of the HPC system	The event will be postponed to another date.
Delay in online event tool	Plenty of flexibility is ensured by online webinars. Different platforms can be selected.
Difficulty in ensuring enough representation from the target stakeholders, namely policy makers, funding agencies and national authorities	The event will be organised in collaboration with, and eventually co-organised, with the FocusCOE initiative and other relevant HPC initiatives. The EC will be involved in the organisation from the very beginning.