31-08-2022

Targeting Real chemical accuracy at the EXascale

D6.2 – First report on the status of organisation of training events and activities, including validation surveys.

Version 1.0

GA no 952165

Dissemination Level

☒ PU: Public
☐ PP: Restricted to other programme participants (including the Commission)
☐ RE: Restricted to a group specified by the consortium (including the Commission)
☐ CO: Confidential, only for members of the consortium (including the Commission)

Document Information

Project Title	Targeting Real Chemical accuracy at the EXascale
Project Acronym	TREX
Grant Agreement No	952165
Instrument	Call: H2020-INFRAEDI-2019-1
Topic	INFRAEDI-05-2020 Centres of Excellence in EXascale computing
Start Date of Project	01-10-2020
Duration of Project	36 Months
Project Website	https://trex-coe.eu/

Deliverable Number	D6.2
Deliverable title	First report on the status of organisation of training events and activities, including validation surveys.
Rev. Due Date	M20 – 31-05-2022
Actual Submission Date	31-08-2022

Work Package	WP6 – Training and User Uptakes
Lead Author (Org)	Ivan Stich (IPSAS)
Contributing Author(s) (Org)	ALL Beneficiaries
Reviewers (Org)	C. Filippi (UT) ; S. Pittonet (TRUST-IT) ; Jan Beerens (UT)
Version	V1.0

Dissemination level	Public
Nature	Report
Draft / Final	Final
No. of pages including cover	48

Disclaimer

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

The content of this document does not represent the opinion of the European Union, and the European Union is not responsible for any use that might be made of such content.

Versioning

Version	Date	Authors	Notes
V1.0	31-08-2022	Ivan Stich	Updating D6.2

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
MPG	MAX-PLANCK-GESELLSCHAFT ZUR FORDERUNG DER WISSENSCHAFTEN EV
UVSQ	UNIVERSITE DE VERSAILLES SAINT-QUENTIN-EN-YVELINES.
Megware	MEGWARE COMPUTER VERTRIEB UND SERVICE GMBH
TUL	POLITECHNIKA LODZKA
TRUST-IT	TRUST-IT SRL
IPSAS	FYZIKALNY USTAV SLOVENSKEJ AKADEMIE VIED (IPSAS)
UPON	UNIVERSITY OF KONSTANZ
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/)

Table of Contents

Document Information 1

Disclaimer 2

Versioning 3

Abbreviations 4

Table of Contents 5

List of Tables 6

1 Introduction .... - 1 -

2 Overview of Training and Education .... - 3 -

2.1 Groups targeted in TREX training activities .... - 3 -

2.2 Training and Education concepts in the M1-M18 period .... - 5 -

3 Internal Training and Education Activities .... - 9 -

3.1 Internal Assessment of Training Needs: WP Kick-Off Meetings .... - 9 -

3.2 Personal Career Development Plan .... - 10 -

3.3 Mentoring and Hosting Researchers .... - 10 -

3.4 University education .... - 11 -

3.5 Specific Training and Education Activities .... - 11 -

4 External Training and Education .... - 13 -

4.1 Events completed/upcoming at the time of writing .... - 13 -

4.2 Planned Events .... - 27 -

5 Impact of events .... - 38 -

5.1 Survey ID020 TREX e-school on QMC with TurboRVB .... - 39 -

5.2 Survey ID012 – Hackathon I .... - 40 -

5.3 ID002 – QMC Hands-on Summer Workshop .... - 41 -

6 Summary and perspectives .... - 43 -

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.

List of Tables

Table 1: Overview of training audience and link to TREX. .... - 3 -

1 Introduction

The TREX Centre of Excellence (CoE) aims at developing, promoting, and maintaining high-performance software solutions in the field of quantum chemistry, computational physics, and materials science, to take advantage of the upcoming exascale architectures. The TREX software platform with its refactored and optimized codes and its challenging state-of-the-art applications, including machine learning (ML) and data analytics, 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.

TREX deals mainly with QMC methods which are among the most accurate, albeit also numerically most expensive electronic structure methods. In combination with their uninhibited scaling with the numbers of CPUs and GPUs, they have the potential to eventually replace in the next 10-15 years the better established and currently much wider used density functional (DFT) and quantum chemistry methods. However, the QMC community is significantly smaller than the DFT and quantum chemistry communities and also the number of corresponding QMC codes. Hence, in order to enable the transition towards QMC methods, a very ambitious training and education program was outlined and is implemented in the TREX CoE.

Thus, one of the key pillars of TREX is the training programme to foster the use of the developed HPC flagship codes by relevant users and to engage and forge a new generation of highly-skilled computational scientists. This is addressed in two specific work packages focused jointly to boost training, education, and user's uptake (WP6) as well as outreach and dissemination of TREX results (WP7). The present document (D6.2 "First report on the status of organisation of training events and activities, including validation surveys") provides a status overview at M20 of the TREX training and education programme, including an assessment and validation of the activities accomplished.

Owing to the ambitious goals, the TREX training and education strategy requires several levels of approach and different groups of instructors and learners. Consequently, several training events, actions, and education efforts have been designed, planned, and implemented in this reporting period. Training events include hands-on workshops for code users and developers, schools, participation to satellite events, hackathons, webinars. Education activities also include university education, hosting students and researchers, mentoring, specific training and education events, etc. Last but not least, as the codes developed in TREX become public, direct support for the code users and developers is also being implemented.

The target audience for TREX training are both code developers as well as well as code users with expertise levels ranging from master students to senior researchers, in academia and industry alike. Special attention is given to the engagement of communities in countries currently developing their HPC facilities and ecosystems. Indeed, the HPC facilities vary appreciably across Europe: generally the "old" EU countries have better HPC systems in operation than the "new" countries, but there are appreciably differences also among those groups (for instance, the Czech Republic or Poland have much better HPC systems than Slovakia). Fortunately, these disparities are partially offset by resource sharing offered across EU, such as PRACE or EuroHPC.

The current document D6.2 describes and details the structure of the training and education strategy and the plans of the events that have taken place at the time of writing and those planned for the remaining project lifetime. Various criteria are used to sort most of the planned activities: distinction is made based on subject (HPC, quantum chemistry), between the planned, upcoming and future events, between events internal to the consortium and events open to an external audiences. The document D6.2 is structured in 6 Chapters. Chapter 2 outlines the overall training and education strategy. Internal training and education activities are described in Chapter 3. The largest section, Chapter 4, describes the activities open to external audiences. Chapter 5 deals with the impact of the events. Chapter 6 gives the summary and perspectives.

2 Overview of Training and Education

In Section 2.1, the target audience is introduced. Training and Education concepts in the M1-M18 period are described in Section 2.2 which also details the consequences on TREX training and education introduced by COVID-19 pandemic and by the Ukraine war.

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 are involved in specific training activities:

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

1. **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.

2. **Trainers.** TREX partners 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 chemistry simulations and HPC applications.

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 Centres
	Students	Undergraduate and PhD university students
	Postdocs	Postdocs at universities and HPC centres
	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

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 TREX activities specifically aim at training a new generation of Computational Science researchers. This effort is extremely beneficial, in particular, in member countries currently developing their HPC know-how and/or infrastructures. TREX training is closely aligned with the EuroHPC strategy and is expected to lead to a higher usage of HPC resources. Such a usage is facilitated by the public availability of training instruments (webinars, lectures, videos) accessible together with TREX software via the TREX website (developed within WP7) and of technical and co-design documentation (which, in part, is already on-line https://www.trex-coe.eu/trex-quantum-chemistry-codes, https://www.trex-coe.eu/trex-quantum-chemistry-libraries). Furthermore, high-level technical support is currently being setup within WP6 to assist the users of the TREX software platform in an optimized exploitation of current and future HPC infrastructures. In this endeavour TREX actively seeks coordination with other CoEs, NCCs, and organizations (e.g., PRACE) on HPC and exascale computing 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 (MaX, MARVEL, and the Swedish in particular).

III. Current and upcoming players beyond the European HPC ecosystem. Some of the technical challenges tackled by TREX both in quantum simulations and in HPC are also common to other related groups and projects in the scientific community worldwide. A good example being, for instance, the ECP (The Exascale Computing Project, https://www.exascaleproject.org) in the U.S.A. which turns around the QMC code that consortium develops (QMCPACK). Hence, a mutually beneficial cross-fertilization is both natural and inevitable. This materializes in several forms. The codes developed by the consortia (for instance TurboRVB and QMCPACK) have been benchmarked head-to-head, an action which is more related to WPs 1-3. More relevant to WP6 is sharing the expertise in training and education. For instance, TREX was present and monitored the QMCPACK Users Workshop 2021 (https://qmc2021.ornl.gov). Vice versa, all the training material developed within TREX is and will be made available on-line for use by the community and to further foster the international collaboration. Good examples are the TREX e-school on Quantum Monte Carlo with TurboRVB (ID020; https://trex-coe.eu/trex-e-school-quantum-monte-carlo-turborvb-recordings-and-presentations) or the QMC Hands-on Summer Workshop (ID002; https://www.trex-coe.eu/events/qmc-hands-summer-workshop-0). A similar practice will be followed also in all future events.

IV. Hardware manufacturers and industrial players (internal and external to TREX). The results of our detailed performance assessment of flagship codes and QMCkl library is of interest to computer manufacturers and already constitutes the basis for collaborations related to hardware and/or software improvements (compiler/OS) as already detailed in D8.3. As regards activities primarily within WP6, some important steps have also been made. We have invited the representatives of SiPearl (https://sipearl.com/en), the EU developer of microprocessors for future EU supercomputers, to our Hackathon II (ID013) to UVSQ. A presentation "Way forward for HPC architectures" was delivered by SiPearl. TREX has collaboration with SiPearl and ATOS (https://atos.net/en/) on the EPI processor. Further collaborations with hardware manufacturers, primarily via UVSQ, include CEA (https://list.cea.fr/en/), INTEL, AMD, ARM, and AWS.

At the time of writing, TREX already collaborated with Sipearl in the framework of the Teratec 2022 conference, where TREX joined the Europa Village organised by the European Commission dedicated to the European HPC ecosystem with a poster co-authored by Sipearl explaining TREX offer for the HPC industrial community. TREX is also in the process of establishing links to TACHYUM (**Error! Hyperlink reference not valid.**), designer of a high-performance high-efficiency universal Prodigy processor, which is expected to find its way also to supercomputers. An attempt will be made to attract a TACHYUM representative to the HPC workshop to take place in Bratislava in Q1 2023 (ID010).

As regards policy stakeholders, funding agencies, and national authorities as target stakeholders for TREX training activities, their invitation to some selected events will be attempted. In particular, they will be invited to the final event (ID005) with the aim of ensuring awareness and uptake of the TREX recommendations.

2.2 Training and Education concepts in the M1-M18 period

TREX training and education strategy as outlined in D6.1 has been essentially followed in the M1-M18 period. We briefly mention below how our training activities were affected by the COVID-19 pandemic and outbreak of the war in Ukraine, and how we addressed these difficulties. The strategy of internal (Sect. 3) and external (Sect. 4) training focussed on both the code end-users (T6.2) and code developers (T6.4) was implemented with high preference given to practical hands-on training. University education is regarded as one of the most effective ways to guarantee that the new generation of students acquires the needed mindset to become active players in the upcoming radical HPC transformations. This was pursued via T6.3. Alongside with development of our TREX software, implementation of user support triage is underway (T6.1). These training activities are summarized in Table 2. In addition, in a less formal way, most TREX partners do teach at the European Universities and use this opportunity to transfer their expertise to university students

Table 2: Overview of the planned events (M-month, Q – year quartile)

Event ID	Event/Action type	Expected period	Actual date	Linked to task	Sect./Page
ID001	Support Triage	M5-M36	Ongoing	T6.1	4.1.1/12
ID002	QMC Hands-on Workshop (IP SAS)	2022 Q1	June 2022	T6.2	4.1.2/14
ID003	Workshop (TUL)	2022 Q4		T6.2	4.3.1/26
ID004	Satellite Hands-on QMC tutorial	2022 Q3		T6.2	4.3.2/27
ID005	Final School	M36		T6.2	4.3.3/27
ID006	Winter School	2021 Q1	January 2021	T6.3	4.1.3/16
ID007	Winter School	2022 Q1	January 2022	T6.3	4.1.3/16
ID008	Winter School	2023 Q1		T6.3	4.1.3/16
ID009	Python Visual QMC application	M5-M36	moved to WP4	T6.3	4.1.4/18
ID010	HPC Workshop (IP SAS)	2023-Q1		T6.4	4.3.4/29
ID011	HPC Workshop (CECAM)	2022-Q4		T6.4	4.3.5/30
ID012	Hackathon I.	2021-Q2	November 2021	T6.4	4.1.5/19
ID013	Hackathon II.	2021-Q4	February 2022	T6.4	4.1.6/21
ID014	Hackathon III.	2022-Q1		T6.4	4.3.6/31
ID015	Hackathon IV.	2023-Q1		T6.4	4.3.7/32
ID016	Webinar	2022-Q4		T7.1	4.3.8/33
ID017	Webinar	2023-Q1		T7.1	4.3.8/33
ID018	Webinar	2023-Q2		T7.1	4.3.8/33
ID019	Final Event	M34		T7.4	4.3.9/36
ID020	e-school on QMC with TurboRVB	2021-Q3	July 2021	T6.2	4.1.7/23
ID021	School on QMC with TurboRVB	2023-Q3		T6.2	4.4.2/35
ID022	CodeRefinery workshop	2022-Q4	November 2020	T6.4	4.1.8/22

2.2.1 Training at the time of COVID-19

Most of WP6 deals directly with education, requiring personal encounters, and was therefore affected by the COVID-19 measures, which rendered the organisation of training and education more complicated. While our original plans for training and education relied on “classical” F2F meetings, COVID-19 advent has forced us to fully reorganize our training and education activities in the first half of the project (M1-M18). At the current stage, the training activities are resuming in the F2F mode again and we hope that they will remain in this mode for the entire second half of the project. As an effect of the COVID-19 measures, some events have been delayed to allow their in-presence organization (e.g. ID002, ID013). Ultimately, the measures imposed by COVID-19 had also some up-sides:

1. The virtual WP6 events have been recorded and a full collection of those videos is available, see the TREX webpage (https://trex-coe.eu/events).
2. Compared to the in-presence meetings, the virtual events eventually attracted more participants as no travel costs were involved. A very good example is the TREX e-School on Quantum Monte Carlo with TurboRVB (ID020) which attracted unprecedented 79 participants.

2.2.2 Effect of Ukraine war on training

At around M17, the war in Ukraine has started. As regards WP6, it is expected to mainly affect events organized in countries directly bordering Ukraine (e.g., PL, SK) which might be perceived, despite geographical distance, as less safe, deterring potential participants from traveling to those countries. The first meeting facing the Ukraine war factor was the event in Slovakia (ID002), which met the target of about 20 young researchers present in person, which were primarily from Slovakia. Deeper assessment of this effect and the increased costs of travel will be possible after analysing more events; the next being in Poland (ID003).

2.2.3 TREX Training and Education Core Team

Table 3 lists the core group of TREX consortium members actively involved in WP6, Training and User uptake. The original crew listed in Table 3 underwent a few modifications. As of May 2022, Mariella Ippolito (CINECA) replaced Fabio Affinito and Niccolò Zazzeri (TRUST-IT) replaced Jacopo Mariani. With deep sadness, we took notice of the serious accident suffered by Sandro Sorella in May 2022 and his passing away in August 2022.

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

Who	Contact point for expertise
Ivan Štich	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
Nizzolò Zazzeri	Dissemination and outreach for training

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 Sect. 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 same goal was also achieved by Hackathon II, described in Sect. 4.1.6, which was also, but not exclusively, an internal training. The career development strategy of partners is summarised in Sect. 3.2. The Collaboration of the researchers and juniors is elaborated on in Sect. 3.3. Implementation within the university educational programme is described in Sect. 3.4. A good example of specific introductory training by our TREX partner, UVSQ, which initiated education and training regarding the code performance evaluation, see below.

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 4) contained a large education component. The presented introductory lectures on quantum chemistry, HPC, and TREX goals were intended so that the members of the TREX team were 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. This, for instance, led to the demand for some specific (originally not planned) training events (e.g., basics of code maintenance, GitHub usage, etc.), now a firm part of TREX. In this respect, the assistance from the CodeRefinery project (see Sect. 4.1.8) was important. Questions were raised frequently and answered by the presenters to the satisfaction of the attendees. Together with the attendee's positive feedback, this confirmed that the kick-off-meeting presentations were generally useful and served their purpose.

Table 4: 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
14-04-2021	Kick-Off Meeting – WP4	Workflows for HTC and HPDA solutions, algorithms and toolkits

3.2 Personal Career Development Plan

Some institutions of the TREX consortium have programs in place to encourage and support their employees to continuously develop their personal and professional careers. They are conceived in accordance with their institutions' rules for career development.

Table 5: Individual Career and Development pages per partner gives links, where available, to the TREX consortium partners' websites explaining the career additional events.

Table 5: 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
MPG	-
UVSQ	-
Megware	Internal Process with process ID M_PB_04 (accessible for all MEGWARE employees)
TUL	https://www.p.lodz.pl/en/hrlogo
TRUST-IT	Part of the Gender and Equality Plan https://trust-itservices.com/gender-equality-plan
IPSAS	-
UKON	-

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.

Junior TREX scientists (postdoc and software engineers) joining the host groups and institutions are of course benefiting from the additional local training and supervision expertise. Furthermore, it is important that the junior scientists benefit from the interconnectivity between the consortium groups and that the training at TREX events and at the host institutions is supplemented by periods spent in the laboratories of the other partners.

Due to the COVID-19 pandemic, such plans have been hampered during the first year. However, already in the last 6 months of the first period, several junior scientists have visited other laboratories within the consortium. Scientifically fruitful exchange visits have already taken place between UT-CNRS/Toulouse, UVSQ-UT, CNRS/Toulouse-UVSQ, CINECA-SISSA, and KTH-SISSA. More are expected in the second period of the project.

The mentoring effort by TREX partners also extends to researchers outside the consortium. For instance, the masters and PhD students, and postdocs of the TREX partners' groups have been joining some of the (internal and external) training events and can therefore access the knowledge and tools and software developed within TREX.

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. We are striving to make sure that the TREX expertise makes its way to the university curricula of the TREX academia partners. At the current stage, it primarily affects chemistry and HPC programmes, followed by condensed matter physics, materials science, and beyond. For instance, the theoretical and hands-on material on QMC we have developed for the Luchon Winter School (ID006, ID007) has been integrated in a new course on Electronic Structure in the Applied Physics program at the UT.

Furthermore, for curricula specialized in HPC (such as the 2 years UP Saclay/UVSQ Master program), TREX developed 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 are used to solve basically the same problem.

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.

Performance evaluation training for code developers

3.5.1 Performance evaluation training for code developers

At the beginning of the TREX project lifetime, the internal TREX code developers have been trained regarding code performance evaluations. The TREX partner, UVSQ, has setup a hands-on training for the code developers during workshops dedicated to each partner and their specific code. The format was 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 have taken place in December 2020 using an online platform. All 6 codes of the 5 TREX partners, see Table 6, were involved.

Table 6: 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

The training sessions consisted of an introduction to the subject, followed by hands-on sessions. The results obtained with the performance tools applied to the partner applications were then presented along with further practical demonstrations on how to use these tools and, in particular, how to deal with the diagnostics they provide. In this respect, Hackathon II, Sect. 4.1.6, was also an important event for in-presence internal education and interaction.

A server (protected and providing secure connections) has been set-up to let each application partner upload a representative/realistic version of their code (https://www.trex-coe.eu/trex-quantum-chemistry-codes). We plan to include a few typical data sets alongside.

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 has, so far, organised one training course on the use of social media. More might be planned according to specific needs raising from the consortium.

3.5.3 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 have registered as teams containing an additional TREX member with more expertise identified as a helper. For more details, see Sect. 4.1.8. Depending on the needs, this procedure may be repeated in the future.

In addition, a training session has been organized for tools used specifically within TREX. Within WP1, org-mode notebooks are used to write a human-readable QMCkl implementation and to maintain consistency between the code and the related documentation. Hands-on sessions have been 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 is in the process of integration in the AiiDa framework. Training in April 2021 was organized, when most of the engineers and post-docs have already started working on the project. These activities have been moved to WP4 as of July 2021.

3.5.3.1 Hackathon II as a mid-term internal training event

Roughly at mid-term, Hackathon II, see also Sect. 4.1.6, was organized as a primarily internal TREX in-presence event. All TREX partners were present with around 40 participants. The hackathon was focused on WP2 and on use and interfacing TREXIO. WP2 leader, Prof. Sorella, presented a lecture on QMC outlooks.

Code efficiency analysis and improvement via MAQAO tools was also demonstrated. Three different codes have been analysed: CHAMP, QP, and TurboRVB. The participants were split into 2 groups which analysed either the molecular codes (CHAMP, QP) or the codes for extended systems (TurboRVB).

All TREX WPs (status, progress, outlooks) have been presented and are available on-line (https://www.trex-coe.eu/events/trex-hackathon-ii-trex-event-uvsq).

4 External Training and Education

Table 2 summarizes events open to external audiences.

The training and education events open to external audience focus primarily on:

1. creation of awareness on the TREX assets
2. fostering the use of the developed codes
3. involvement of the future-generation of HPC ecosystems.

The following Sections are divided into events completed/upcoming at the time of writing (Sect. 4.1), planned events (Sect. 4.2).

4.1 Events completed/upcoming at the time of writing

For each of the completed events or events under active preparation at the time of writing, all the available details are provided below. Additional details can be found via webpage links to the TREX webpage (https://trex-coe.eu/events).

4.1.1 ID001 – Ongoing. Support Triage

At the time of writing, the TREX codes are entering the stage where they will become publicly available via the TREX platform (https://www.trex-coe.eu/trex-quantum-chemistry-codes). This is already the case for NECI, GAMMCOR, QMC = Chem, and Quantum Package. CHAMP and TurboRVB will follow soon.

Codes becoming publicly available are expected to jump the number of users and the probability that they will need support either due to domain-specific issues, improper use of the codes, or potential bugs in the codes (such kind of support will be offered by the code owners). Users may also need support to maximize the TREX codes performance on different architectures, which may require optimization of the computational setup and/or of the code parameters that minimize the time to achieve the solution (this support may be offered by both code owners and HPC specialists).

The support, which follows the good practices adopted for supporting also other publicly accessible computer codes, is in the process of implementation and is expected to be activated in the last quarter of 2022.

The support to the users goes via a single-point of contact (SPC) offered via the main TREX website. This consists of an email address to which all the requests for assistance are conveyed and the email will trigger the creation of a truble ticket in a ticketing system. The tickets received will be classified according to their required level of assistance and the kind of help needed.

The support triage will be operated by an Operator-On-Duty (OOD), and a "trouble ticket" will be assigned to an expert (who could be a code expert or a person working in one of the computing centres). 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 the 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.

Task Scope	
Work Package	WP6 Training and user uptake
Event ID	ID001
Task	T6.1
Task Title	Technical support for the use of TREX codes
Task Responsible	Lead: F. Affinito/Mariella Ippolito – 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 Summer Workshop (IP SAS)

This event was the first TREX workshop organized as an in-presence event. Due to the COVID-19 measures, a later date than initially planned, June 2022, was selected as a safe date. A quiet location in a manor house about 100 km from the capital, Bratislava, (https://kastielmojmirovce.sk/en/), far away from the clutter of large cities was selected. While no restrictions were imposed, the primary target were participants from the local countries, primarily PhD. students, postdocs, and young researchers. 47 participants have registered for the event and, based on their CVs, 29 were selected for participation. 9 selected participants could not come (travel cost, visa problem, Ukraine war, etc.) and were only present online. The Slovakia location for the workshop was selected also to approach the local electronic structure computational community and, accordingly, 9 out of 20 participants (45%) were Slovak. 14 hours of lectures and 12 hours of hands-on training was provided. The workshop carried a clear mission to attract the target group, typically from the DFT/quantum chemistry communities to the alternative accurate and numerically efficient QMC modelling. TREX lecturers from molecular science (C. Filippi, A. Scemama), materials science (M. Casula, K. Nakano, I. Stich, J. Brndiar) and machine learning (A. Tirelli) were present. The presentations are on-line. More details can be found in Sect. 5.3. Participants surveys (Sect. 5.3), suggest that the event was a huge success and served the intended purpose very well.

Photo of participants of the QMC hands-on Summer workshop at Mojmírovce, Slovakia.

Event Overview			
Event ID	ID002	Event Linked	ID010
Event Title	QMC Hands-on Summer Workshop	Event Period	2022-Q2
Event Type	Workshop	Event Date	June 20-23, 2022
Event Location	Slovakia	Event Country	Slovakia
Event Coordinator	Ivan Stich	Event Organisation	IP SAS
Event Description	ID002-T6.2 Workshop IP SAS (manor house Mojmírovce) 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: I. Stich – IP SAS; S. Moroni – SISSA
Event Objectives	Description
Basic QMC training	Crash-course in practical electronic structure QMC theory and computations (16 hours).
Basic TREX code/s hands-on training	Practical entry-level QMC hands-on sessions using TREX codes (QP, CHAMP, TurboRVB). VMC, DMC, for molecules, solids in the domain of molecular and materials science. (12 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: 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 in person plus 9 online
Pre-Requirements	Detail what is required before
codes ready for use	The universal TREX I/O library 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.
Web link	https://www.trex-coe.eu/events/qmc-hands-summer-workshop-0

4.1.3 ID006 – ID007 – ID008 Winter schools

This series of activities targets the youngest audience, master and 1st-year PhD students, and has a form of satellite events to the Luchon Winter School of the Erasmus Mundus Joint European Master Degree program in Theoretical Chemistry and Computational Modelling. These include lectures in theoretical foundations as well as hands-on experience using mostly simplified educational molecular codes. The students are also encouraged to write a simple QMC code by themselves. The first event (ID006) in this series was organized in January/February 2021 and the next (ID007) again in January/February (24. January to 4 February) 2022. Given the dates (winter 2021, 2022), due to the COVID-19 pandemic measures, both events could only be organized in virtual form. Yet, the first event attracted 23 and the second 40 students, which we regard as a success. ID008 is envisaged to take place in 2023 in-presence form.

Event Overview			
Event ID	ID006	Event Linked	-
Event Title	Tutorials in Theoretical Chemistry	Event Period	2021-Q1
Event Type	Satellite Event	Event Date	25. Jan. – 8. Feb
Event Location	Luchon Winter School of the Erasmus Mundus Joint European Master Degree program in Theoretical Chemistry and Computational Modeling	Event Country	virtual
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; I. Stich – IP SAS
Event Objectives	Description
Basic QMC Training	The "Tutorials in Theoretical Chemistry" Luchon Winter School focus 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 participated by teaching one extra day to introduce the basic concepts of QMC methods and to explain the art of writing 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: 23 participants.

	Note: Usually the numbers are larger, however, due to the COVID measures the organizers had to limit the number of the Erasmus Mundus Students due to the difficulties in organizing effective online hands-on sessions for a 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	Democratization of QMC methods. If QMC is learned at the master's degree, it will be considered by young researchers as a wellestablished method and not as an exotic method for a small community of experts.
Related Document	Description
Web page	https://www.irsamc.ups-tlse.fr/lttc https://trex-coe.eu/events/luchon-winter-school

4.1.4 ID009 – Python visual QMC application

This task was originally covered by Dr. Dubecký (STU), who left the project at an early stage, and IP SAS, the successor to STU, plays only a minor role in this activity. The task was moved to WP4 and, accordingly, this activity is reported as a part of WP4.

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	Matúš Dubecký	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 the generation 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 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.

4.1.5 ID012 Hackathon I

In the first period of the project, we have observed that one of the weaknesses of the flagship codes was their installation procedure. This prompted us to organise a "Build system Hackathon" in November 2021. The event was also open to external participants, to offer training on Autotools and Cmake and to provide the help with introduction of these tools within the codes. This hackathon had a large impact on the target TREX codes: CHAMP, TurboRVB, QMC=Chem and GammCor have significantly improved their Autotools or Cmake files. In addition, the preparation of this hackathon forced the teachers to improve deeply their knowledge of these tools, and this had also a strong impact on the build systems of the libraries that they develop within TREX, namely QMCkl and TREXIO. This training was also beneficial to the external attendees who obtained the same benefits as TREX participants. 8 plenary main topics were covered, 4 hands-on tutorials were organized. 4 TREX codes (CHAMP, QMC=Chem, TurboRVB, GammCore) and 3 other (participants' codes). 51 live attended were present, 22 selected for hands-on tutorials. All lectures are online as YouTube presentations. More details, including participants' surveys are in Sect. 5.2. The surveys suggest a high-level of satisfaction.

Event Overview			
Event ID	ID012	Event Linked	-
Event Title	TREX Hackathon I.	Event Period	2021-Q4
Event Type	Hackathon	Event Date	November 8.-12.
Event Location	virtual	Event Country	virtual
Event Coordinator	A. Scemama	Event Organisation	CNRS
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 Cmake, Autotools
Org-mode	Literate programming Reproducible research
Programming with IRP	What is IRP programming Hands-on session
Cmake, Atotools	Hands-on session
Event Target Audience	Description of audience and expected number of participants, entry level

Code owners, new developers, university students	7 codes, 4 TREX codes 51 attendees, 22 selected for hands-on tutorials
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 code developers will become proficient with the common tools
Web link	https://trex-coe.eu/events/trex-build-system-hackathon-8-12-nov-2021

4.1.6 ID013 – Hackathon II.

Hackathon II was an internal TREX event, see also Sect. 3.5.4, opened also to external audiences. Due to the COVID-19 pandemic restrictions, this event was the first WP6 event taking place in-presence mode and it was also the first TREX event where the TREX partners could meet in person. All TREX partners were present. The number of participants was around 40. The hackathon was focused on WP2 and on use and interfacing TREXIO. WP2 leader, Prof. Sorella, presented a lecture on QMC outlooks. Code efficiency analysis and improvement via MAQAO tools was demonstrated. Three different codes have been analysed: CHAMP, QP, and TurboRVB. The participants were split into 2 groups which analysed either the molecular codes (CHAMP, QP) or the codes for extended systems (TurboRVB). All TREX WPs (status, progress, outlooks) have been presented and are available on-line (https://www.trex-coe.eu/events/trex-hackathon-ii-trex-event-uvsq). Hardware manufacturers were represented in Hackathon II by SiPearl, see also Sect. 2.1. The webpage also contains a link to the YouTube interview of William Jalby, the organizer of the event, who speaks about the Hackathon.

TREX
Targeting Real chemical accuracy at the EXascale

A teaching moment at the TREX Hackathon II in Versailles, France

Event Overview			
Event ID	ID013	Event Linked	-
Event Title	TREX hackathon II.	Event Period	2022-Q1
Event Type	Hackathon	Event Date	February 28—March 4
Event Location	UVSQ	Event Country	France
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 event targeted developers mainly from within the TREX who learned the art of code efficiency analysis and improvement via MAQAO tools. Three different codes have been analysed: CHAMP, QP, and TurboRVB. The participants split into smaller groups.
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 1. Vectorisation 2. Memory hierarchy 3. Scalability 4. 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
Web link	https://trex-coe.eu/events/trex-hackathon-ii-trex-event-uvsq

TREX
Targeting Real chemical accuracy at the EXascale

Photo of participants at the TREX Hackathon II in Versailles, France.

4.1.7 ID020 TREX e-school on QMC with TurboRVB

ID020 was initially included in the training plan as an "Additional Event". This virtual event attracted an unusually large number of participants (89 live attendees) which, due to practical restrictions, had to be limited to 24 in the hands-on sessions. 18 hours of lectures (A. Sorella, M. Casula, K. Nakano) and 8 hours of hands-on training (K. Nakano) were provided. All material is online via TREX webpage. The plans are to organize this event biannually, i.e., the next one in 2023, see also Sect. 4.2.9. More information, including participants' surveys are in Sect. 5.1. Based on the surveys, this event was extraordinarily successful.

Event Overview			
Event ID	ID020	Event Linked	-
Event Title	TREX e-school on QMC with TurboRVB	Event Period	2021-Q3
Event Type	Workshop	Event Date	July 12-16, 2021
Event Location	virtual	Event Country	virtual
Event Coordinator	Sandro Sorella	Event Organisation	SISSA
Event Description	ID020-T6.2 Workshop SISSA, Italy		

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: Sandro Sorella – SISSA; S. Moroni – SISSA
Event Objectives	Description
Basic QMC training	Crash-course in practical electronic structure QMC theory and computations (18 hours).
Basic TREX code/s hands-on training	Practical entry-level QMC hands-on sessions using TurboRVB TREX code. VMC, DMC, for 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: 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: 89 (limited to 24 in the hands-on training)
Pre-Requirements	Detail what is required before
codes ready for use	TurboRVB codes debugged for the tasks described in event objectives.
Impact after event	Detail what impact is targeted
Increased QMC awareness	Most of the expected participants did not have any experience with QMC. Their participation has increased the number of members of the “QMC-aware” community.
New QMC users	An increased number of QMC users 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 did have chance to interact with TREX codes, participants already using QMC in their research had chance to find better solutions for their research.
Web link	https://trex-coe.eu/events/trex-e-school-quantum-monte-carlo-turborvb

4.1.8 ID022 CodeRefinery workshop

At the beginning of the project (Nov. 17-19, 2020), TREX participated in a Code Refinery training organised by the Nordic e-Infrastructure Collaboration where the TREX members have been taught the good practice in the collaborative code development (Git/GitHub, code review, continuous integration, ReadTheDocs, etc). TREX partners registered as a group to online course with about 90 participants. See also Sects. 3.1 and 3.5.3.

Event Overview			
Event ID	-	Event Linked	-
Event Title	CodeRefinery workshop	Event Period	2020
Event Type	Workshop	Event Date	Nov. 17-19
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. Learn 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

4.2 Planned Events

In this Section, a concise list of planned events is given. For each of the planned events, all details available at the time of writing of this document are provided. Since many details of the event, such as the precise date, or even precise program, may not be available until about 6 months ahead of the event, such information is not indicated, if unknown.

4.2.1 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: I. Stich – IP SAS; S. Moroni – SISSA
Event Objectives	Description
Training in Quantum chemistry	Practical electronic structure course with focus on Quantum chemistry methods using GammCor and possibly NECI codes in molecular science.
Machine Learning	Focus on how to use the TREX platform together with the machine learning (ML) tools in the domain of molecular 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	The universal TREXIO library operable with TREX codes (GammCor/NICI) and debugged for the tasks described in event objectives
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.

4.2.2 ID004 – Satellite Hands-on QMC tutorial

This event was under preparation since early September 2021 as a satellite to the CESTC (Central European Symposium on Theoretical Chemistry) 2022. Since this is a quantum chemistry symposium, we prepared a tutorial in molecular chemistry. Molecular codes (CHAMP, QP) have been selected for hands-on training to be conducted by the respective code owners, C. Filippi and A. Scemama. Due to the COVID-19 pandemic measures, the CESTC was cancelled twice in 2020 and 2021. It will finally take place in 2022 on 7-10 Sept. in Balatonszarszo, Hungary (https://cestc2022.mke.org.hu/). While the Hungarian CESTC 2022 organizers expressed initial interest in our proposed 1-day extension of the main event and the program we proposed, their later slow response forced us to cancel this event. Since from the discussion with the future CESTC symposia organizers, it is not clear at the time of writing if the next CESTC meeting will indeed take place in 2023, we have decided to replace ID004 by ID021 which, initially, was included in the training plan as an “Additional Event”.

4.2.3 ID005 Final school

The aim of this event is to promote the use of all TREX codes within academia and industry and thus significantly enlarge the QMC user community.

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: I. Stich – IP SAS; 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.

4.2.4 ID010 – HPC Workshop (IP SAS)

This event is expected to be linked with internal TREX member meeting, as in Hackathon II (ID013).

Event Overview			
Event ID	ID010	Event Linked	-
Event Title	TREX HPC Workshop	Event Period	2023-Q1
Event Type	Workshop	Event Date	tbd, 2-3 days
Event Location	Bratislava	Event Country	Slovakia
Event Coordinator	Ivan Stich	Event Organisation	IP SAS, 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; M. Ippolito – 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)

4.2.5 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	M. Ippolito	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; M. Ippolito – CINECA
Event Objectives	Description
Code development training	The objective of this event is to train 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 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)

4.2.6 ID014 – Hackathon III.

Event Overview			
Event ID	ID014	Event Linked	-
Event Title	TREX hackathon III.	Event Period	2022-Q4
Event Type	Hackathon	Event Date	tbd
Event Location	Bologna	Event Country	-
Event Coordinator	M. Ippolito, 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; M. Ippolito – 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.

4.2.7 ID015 – Hackathon IV.

Event Overview			
Event ID	ID015	Event Linked	-
Event Title	TREX Hackathon IV.	Event Period	2023-Q1
Event Type	Hackathon	Event Date	tbd
Event Location	Megware	Event Country	Germany
Event Coordinator	A. Auweter	Event Organisation	Megware
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; M. Ippolito – 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

4.2.8 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. Three webinars will be organised with target scope and structure: one to present the contribution of TREX to the HPC ecosystem, co-organised with partner CoE initiatives Max, NOMAD and CO2; a second one targeting the benefits for industry, organised in collaboration with Megware and Sipearl and engaging other relevant industrial actors; a third one aimed at showcasing TREX demonstrators to a scientific audience.
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 three webinars will be organised according to the tentative timeframe below: • 2022-Q4 - October/November 2022: TREX in the HPC ecosystem • 2023-Q1 - February/March 2023: - TREX offer for the European Microprocessors Industry • 2023-Q2 - May/June 2023: TREX Demonstrators

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.

4.2.9 ID021 TREX school on QMC with TurboRVB

The event ID021 will closely mirror event ID020, the main difference being that it now planned in presence form. This event is proposed as a replacement for ID004, Sect. 4.2.2.

Event Overview			
Event ID	ID021	Event Linked	-
Event Title	TREX e-school on QMC with TurboRVB	Event Period	2023-Q3
Event Type	Workshop	Event Date	
Event Location	Trieste, Italy	Event Country	Italy
Event Coordinator	Sandro Sorella	Event Organisation	SISSA
Event Description	ID021-T6.2 Workshop SISSA, Italy		

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: Sandro Sorella – SISSA; S. Moroni – SISSA
Event Objectives	Description
Basic QMC training	Crash-course in practical electronic structure QMC theory and computations (18 hours).
Basic TREX code/s hands-on training	Practical entry-level QMC hands-on sessions using TurboRVB TREX code. VMC, DMC, for 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: 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: around 20
Pre-Requirements	Detail what is required before
codes ready for use	TurboRVB codes debugged for the tasks described in event objectives.
Impact after event	Detail what impact is targeted
Increased QMC awareness	Most of the expected participants are expected not have any experience with QMC. Their participation will increase the number of members of the “QMC-aware" community.
New QMC users	An increased number of QMC users 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.

4.2.10 ID019 Final Event

Final event, listed in Table 2, while important for the TREX project is not a training event and will not be described here. It will be covered under WP7.

5 Impact of events

The outcomes (results and consequences) of the TREX training and education events and actions implemented in WP6 are briefly summarized in Table 7. The detailed outline can be found in Sects. 3 and 4. Perhaps the most important outcome is related to use of the software developed and maintained by the TREX consortium. Detailed information on statistics of TREX software use will be collected after all the TREX codes go public (https://www.trex-coe.eu/trex-quantum-chemistry-codes) and the unique cloners will be determined via Github/Gitlab facilities. Our preliminary statistics indicate about 18 unique cloners of QP (Github) and 21 of TurboRVB (Gitlab). These numbers are expected to increase sharply after the TREX software goes fully public.

Table 7: Brief Summary of the actual outcomes of the TREX training and education program.

Type	Explanation
TREX code user uptake	Increase in number of TREX users via events (schools, workshops, satellite events, hands-on sessions): 89 end-users have been trained, 24 with hands-on TurboRVB experience (ID020); 29 end-users have been trained, 24 with hands-on tutorials with a wider range of TREX software: QP, CHAMP, TurboRVB TurboRVB (ID002). In 6 events (ID002, ID006, ID007, ID012, ID013, ID020) TREX software was used as a teaching tool. Preliminary statistics indicate 18 new QP and 21 TurboRVB users.
TREX code developer's uptake	Two hackathons have been organized one on code installation procedures (ID012) with 51/22 participants/hands-on attendees and one on general code optimisation, including QMCkl and TREXIO (ID013) with about 40 participants.
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 is receiving more attention via training and education. Specifically, the QMC hands-on Summer workshop (ID002) and HPC workshop (ID010) have/will both be organized in Slovakia with still critically underdeveloped HPC ecosystem. In ID002 ≈30% of participants were local. Communication and dissemination channels for creating awareness are addressed by WP7 increase the impact further.
Higher and effective use of current and upcoming HPC infrastructures	Most of the electronic structure software (DFT, GW, quantum chemistry) is not suited for the challenges posed by the upcoming HPC infrastructure. TREX training and education program promoting the stochastic QMC alternatives is significantly changing the situation via the code user (ID002, ID020) and code

	developer (ID012, ID013) uptake. These and future TREX events already did and will enlarge the pool of experienced users and developers of stochastic quantum software ready for future-generation of HPC infrastructure.

Validation of completed events

For a selected subset of completed events an explicit validation, including participants surveys after the event, was conducted. This was done by TRUST-IT as a part of the WP7 activities.

5.1 Survey ID020 TREX e-school on QMC with TurboRVB

General information:

- **5** days e-School/workshop
- **10** Plenary main topics
- **1** Hands-on tutorial each day
- **5** Expert speakers
- **1** TREX code (TurboRVB)

- **33 Countries represented**
  - **22 – India**
  - **10 – Italy**
  - **7 – United States**
  - **6 – France**
  - **4 – China**

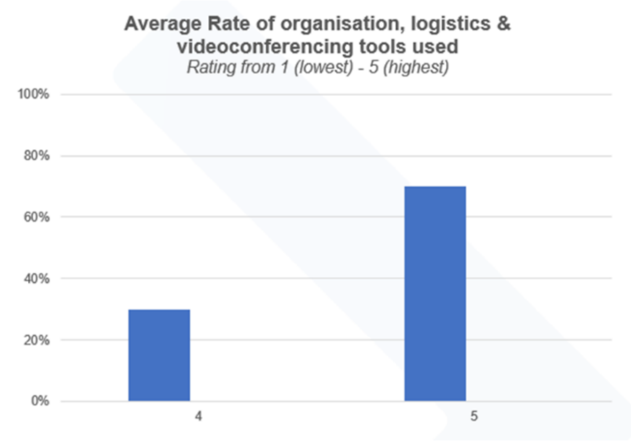
- **Participants**
  - **94** Valid participants
  - **24** Chosen for Hands-on attendees
  - **89** Live attendees

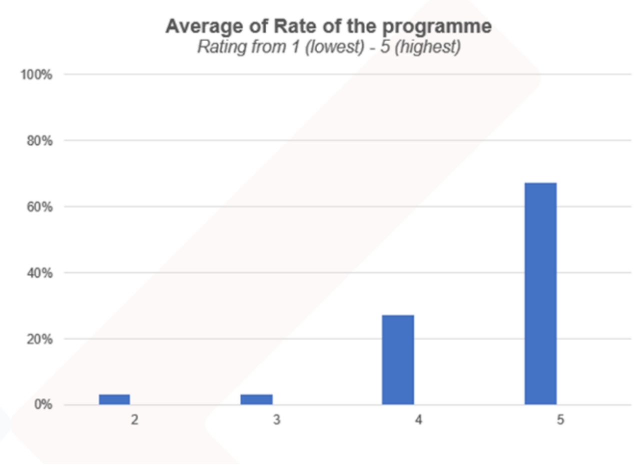
- **Stakeholder Type**
  - **83%** Academia
  - **11%** Players beyond the European HPC ecosystem
  - **4%** European HPC ecosystem
  - **2%** **H**ardware manufacturing & industrial players

- **Gender** ♂ **83%** ♀ **17%**

Survey:

- **Survey Results**
- **30 Respondents**





5.2 Survey ID012 – Hackathon I

General information:

- **4** days Hachathon I
- **8** Plenary main topics
- **1** Hands-on tutorial each day
- **11** Expert speakers and tutors
- **3 TREX codes** (CHAMP, TurboRVB, Gammcor)
- **3 other codes** (Quack, Cmake and Autotools)

- **Participants**
  - **51** Participants
  - **22** Chosen Hands-on attendees
  - **51** Live attendees

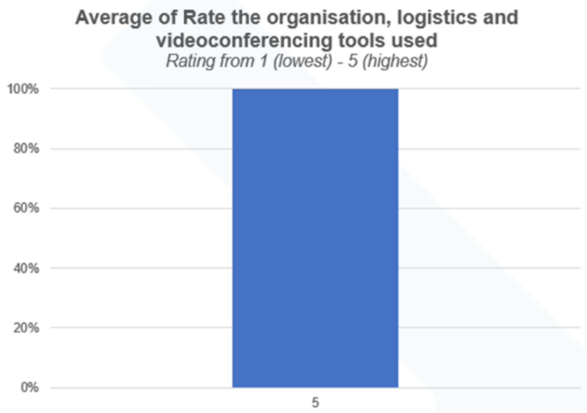
- **Stakeholder Type**
  - **61%** Academia
  - **24%** European HPC ecosystem
  - **8%** Hardware manufacturing
  - **8%** Players beyond the European HPC ecosystem

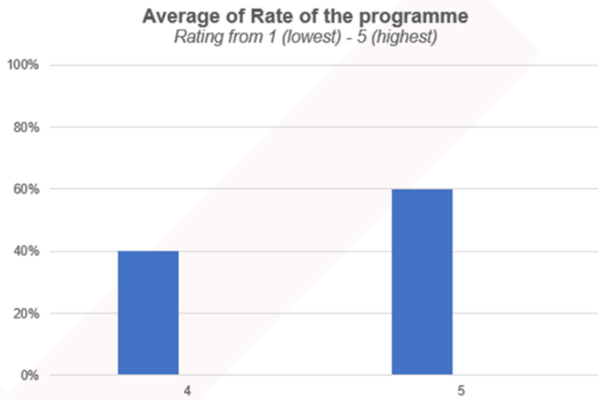
- **21** Countries represented
  - **13 – France**
  - **6 – India**
  - **6 – Italy**
  - **4 – Germany**
  - **4 – Poland**

- **Gender** ♂ **90%** ♀ **10%**

Survey:

- **Survey Results**
- **5 Respondents**





5.3 ID002 – QMC Hands-on Summer Workshop

General information:

- **4** days Summer workshop
- **3** Plenary main topics
- **5** Hands-on topics and applications
- **8** Expert speakers and supports
- **3** TREX codes (TurboRVB, Quantum Package, CHAMP)

- **Participants**
  - **47** Registered participants
  - **29** Chosen students
  - **20** Live attendees
  - **9** Online attendees

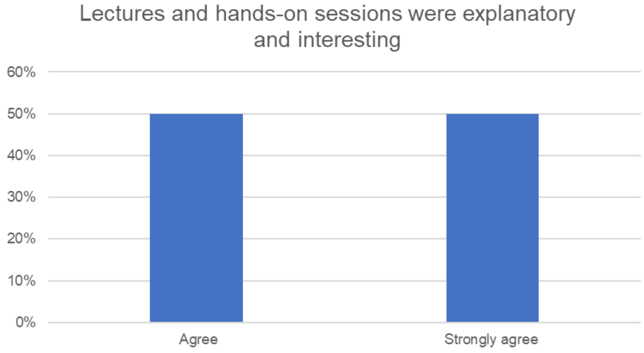
- **Stakeholder Type**
  - **100%** Academia

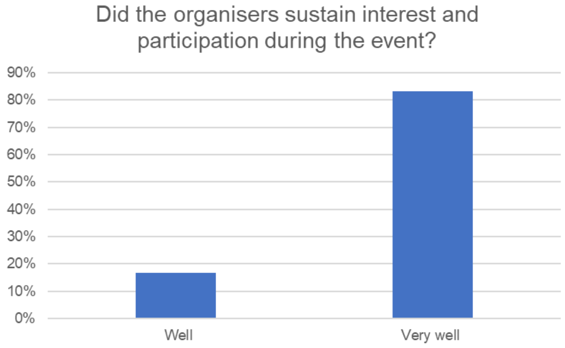
- **18** Countries represented
  - **9** Slovakia
  - **5** Italy
  - **4** France
  - **2** Germany
  - **2** India

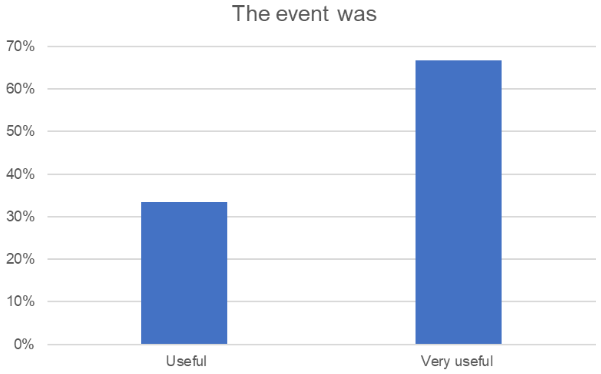
- **Gender** ♂ **76%** ♀ **24%**

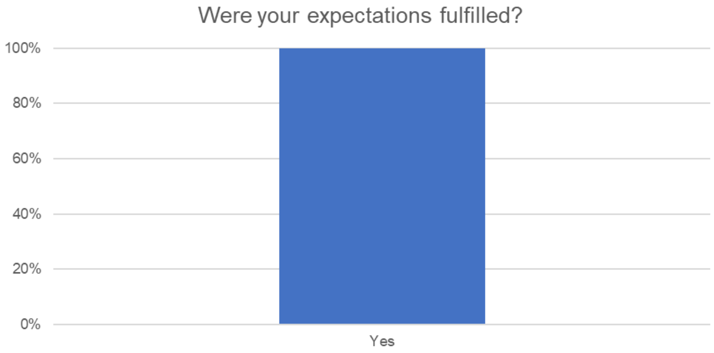
Survey:

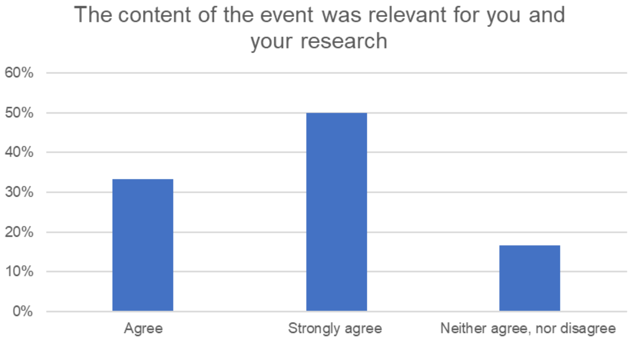
- **Survey Results**
- **9 Respondents**


Lectures and hands-on sessions were explanatory and interesting
60%
50%
40%
30%
20%
10%
0%
Agree
Strongly agree


Did the organisers sustain interest and participation during the event?
90%
80%
70%
60%
50%
40%
30%
20%
10%
0%
Well
Very well


The event was
70%
60%
50%
40%
30%
20%
10%
0%
Useful
Very useful


Were your expectations fulfilled?
100%
80%
60%
40%
20%
0%
Yes


The content of the event was relevant for you and your research
60%
50%
40%
30%
20%
10%
0%
Agree
Strongly agree
Neither agree, nor disagree

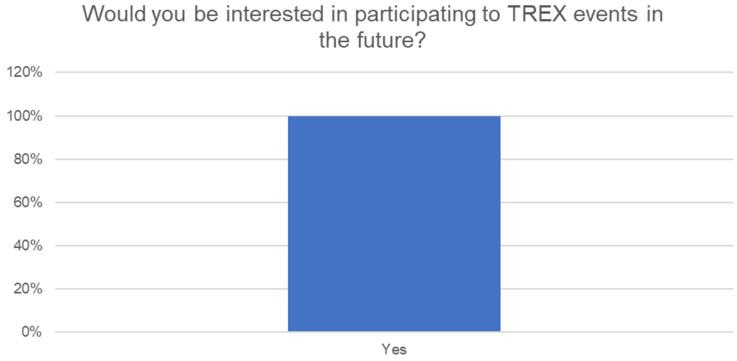

Would you be interested in participating to TREX events in the future?
120%
100%
80%
60%
40%
20%
0%
Yes

Photo of a hands-on session (A. Scemama lecturing) at QMC hands-on summer workshop at Mojmírovce, Slovakia.

6 Summary and perspectives

In summary, the document D6.2 provides an overview of the general training and education strategy implementation within WP6 and of its current achievements. This covers audience types, overview of events with a timeline, and details of all events, completed, on-going or planned, internal and those opened to external audiences, as known at the time of writing.

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 by WP7 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 deliverable is scheduled to be provided within the project duration:

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

Future work includes the organization of individual events as well as of the related post-event measures (preparation of reports with validation surveys, summary, etc.).