



D7.4 – Communication, dissemination, and stakeholders engagement interim report, and user uptake updates

Version 1.0

GA no 952165

Dissemination Level

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Abbreviations

Abbreviation	Translation
CECAM	CENTRE EUROPÉEN DE CALCUL ATOMIQUE ET MOLÉCULAIRE
CINECA	CINECA CONSORZIO INTERUNIVERSITARIO
CNRS	CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE
CoE	CENTRE OF EXCELLENCE
CSA	COORDINATION SUPPORT ACTION
EU	EUROPEAN UNION
F2F	FACE-TO-FACE
HPC	HIGH PERFORMANCE COMPUTING
HPC3	HPC CENTER OF EXCELLENCE COUNCIL
HPDA	HIGH PERFORMANCE DATA ANALYTICS
KPI	KEY PERFORMANCE INDICATOR
ML	MACHINE LEARNING
NCC	EUROPEAN NATIONAL COMPETENCE CENTERS
PRACE	PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE
Psi-k	AB INITIO (FROM ELECTRONIC STRUCTURE) CALCULATION OF COMPLEX PROCESS IN MATERIALS
QMC	QUANTUM MONTE CARLO
SISSA	INTERNATIONAL SCHOOL FOR ADVANCED STUDIES
TREX	TARGETING REAL CHEMICAL ACCURACY AT THE EXASCALE
UT	UNIVERSITEIT TWENTE
UVSQ	UNIVERSITÉ DE VERSAILLES-SAINT-QUENTIN-EN YVELINES
WP	WORK PACKAGE



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Executive Summary

The document is a direct output of WP7 whose key role in the project is to raise awareness about project results, disseminate major outputs, and engage key stakeholders. The aim of this document is twofold:

- It gives an overview of the implementation plan to engage the EU stakeholder community on HPC for stochastic quantum chemical simulations.
- It demonstrates the impact generated by the different activities carried out so far, linking them to the main outputs produced by the TREX project.

This report outlines the communication, dissemination and engagement objectives and actions in the period up to March 2022 (M18). The document provides information on how the project has targeted the main target stakeholders through various channels such as the TREX website, social media, events, schools, and workshops. The document also reports on quantitative and qualitative measures demonstrating the impact of the project.

The first part of this document introduces the impact of the activities deployed by the TREX project (Chapter 1) and how the key exploitable results have been promoted so far (Chapter 2). Chapter 3 reports on the impact of TREX community building through events, training, workshops, and third-party events. Chapter 4 details how TREX interfaced with the HPC ecosystem, while Chapter 5 covers the strategy for impact assessment for communication and dissemination activities for the upcoming months.

The entire deliverable is to be considered as a living document that might slightly change in accordance to the advancements and needs of the other Work Packages, in particular the ones directly involved in the elaboration of the project technical assets (namely, WP1, WP2, WP3, WP4, and WP5). Furthermore, the overall unfolding of the Covid-19 situation might steer the direction of the Communication in different directions, as better indicated in the conclusive part of the document (Chapter 6).



1. Main Achievements from M1-M18

WP7 is responsible for the overall dissemination and engagement activities, including key performance indicators (KPIs) to measure tangible impacts of TREX solutions in the European high performance computing (HPC) context and beyond. The overall goal of the TREX communication, dissemination, and stakeholder engagement plan is to guarantee an effective and road-reach strategy to successfully disseminate TREX exploitable results to the targeted stakeholders throughout the entire duration of the project. The WP7 activities undertaken until M18 and planned for the upcoming months are part of a collaborative effort of all TREX partners, and closely connected with the training and educational activities of WP6. Working relationships with peer HPC Centers of Excellence (CoE) and the FocusCoE CSA have also been important in this phase to boost outreach, improvement, and reuse of the TREX solutions.

In the first 18 months of TREX, some foundational outcomes have been achieved:

- The building of a **widely acknowledged personalised project branding** and visual identity that makes the project recognisable within the European HPC community.
- A seamless engagement of a **broad community of stakeholders** that encompasses early career professionals and senior influential scientific and research actors within the European context.
- A wide **social media channel community** that plays a key role in the solid junction between the project, end-users, and overall community: this is the breeding ground to share most significant insights, newsworthy items, TREX training and outreach events, and participation to other HPC related events.
- The creation of a **fully-fledged, and continuously improved, website** as the core of its communication strategy to showcase the main features of the projects, as well as a safe repository of documents and deliverables.

Quantum Monte Carlo (QMC) approaches at the core of TREX are among the few methods in the field of quantum simulations that can fully exploit the massive parallelism of upcoming exascale supercomputers. The marriage of these advanced methods with exascale will enable simulations at the nanoscale of unprecedented accuracy, targeting a fully consistent description of the quantum mechanical electron problem for very large systems.

Indeed, in the USA, QMC is strongly promoted by national funding agencies, including specific support to take advantage of forthcoming exascale facilities. In Europe, a lively community of QMC practitioners has developed over the years several codes, each featuring some of the most innovative and performing solutions worldwide. The challenge of porting this unique know-how to a new generation of computer architectures is a tremendous opportunity for the European QMC community to:

- join forces to maintain and strengthen its leading profile in the quickly evolving, highly competitive development of QMC;
- deploy the power of top-class, high-end algorithms, jointly with upcoming hardware architectures, to tackle relevant problems in molecular and material science, fundamental physics and chemistry, and artificial intelligence methods.

TREX has started the ground-breaking potential of establishing a QMC-based computational environment, which will be further discussed in Section 2. With the foundations set within this initial period, the community will experience significant advancement in the TREX flagship codes, QMCKl and TREXIO libraries, and TREX demonstrators, which will be disseminated through the channels mentioned in this strategy document.

2. Promotion and dissemination of TREX results & assets

The promotion of TREX results is at the core of the project dissemination plan and its activities. In this Section, we will detail how the activities listed below have been promoted and disseminated.

2.1. TREX real-life demonstrators

A series of challenging exascale-enabled demonstrations are being designed and run to test the readiness and effectiveness of TREX software into real exascale use cases in the field of materials for energy conversion, water description, quantum magnetism and high-temperature superconductor and functional materials. Already at the initial design phase for the project website, it was decided to create 4 dedicated pages for the 4 different demonstrators in TREX, with direct access from the main menu and highlighted in the homepage.


During this reporting period, promotion of the main purpose and scope of these demonstrators took place across TREX social channels with the intent to introduce them to the users.





Figure 1 Sample post about TREX demonstrators

Demonstrators were publicly presented for the first time during the TREX meeting organised on 2-3 March 2022 at the Université de Versailles-Saint-Quentin-en-Yvelines (UVSQ). Michele Casula, IMPMC, Sorbonne Université and CNRS, Ivan Stich, Slovak Academy of Science and Kasia Pernal, Lodz University of Technology, presented how TREX software has been tested so far in real pre-exascale demonstrations. Their presentations and have been published on the TREX Hackathon II event page (<https://www.trex-coe.eu/events/trex-hackathon-ii-trex-event-uvsq>) to be further promoted with the general public.



SAPT: summary

$$\underbrace{\{\gamma, \Gamma\}}_{\text{ERPA}} \rightarrow \underbrace{\begin{pmatrix} A & B \\ B & A \end{pmatrix} \begin{pmatrix} X_\nu \\ Y_\nu \end{pmatrix}}_{\text{ERPA}} = \omega_\nu \underbrace{\begin{pmatrix} N & 0 \\ 0 & -N \end{pmatrix} \begin{pmatrix} X_\nu \\ Y_\nu \end{pmatrix}}_{\text{ERPA}} \rightarrow \underbrace{\{\gamma^{0\nu}, \Gamma^{0\nu}, \omega_\nu\}}_{\text{SAPT}} \downarrow E_{\text{int}}^{\text{SAPT}}$$

Summary: TREXIO use in GammCor

- 1e and 2e integrals read in AO, transformed to NO
- 1-, 2-RDMs read in MO, transformed to NO
- TREXIO tests on CIPSI wave functions from Quantum Package

Figure 2 Presentation by Kasia Pernal (TUL) at the TREX meeting in Versailles

An interview with Michele Casula (IMPMC, Sorbonne Université and CNRS) was also run and will be published in April 2022.



Figure 3 Image from the interview with Michele Casula, CNRS, at the TREX Hackathon II in Versailles, 3 March 2022

For the next period, we foreseen the following dissemination activities specifically related to the TREX demonstrators:

Table 1 Upcoming dissemination activities related to the TREX demonstrators

Activity	Description	M18	M21	M24	M27	M30	M33	M36
Interviews	Interviews with demonstrator owners	1	1	1	1			
Social media promotion	Post targeting demonstrators	continuous						
Revamped demonstrator pages	Updated pages with expanded information about the demonstrators, presentations and accompanying materials		1	1	1	1		
Informative animated video	1 video about the TREX demonstrators			1				
Publications	New scientific publications issued about the demonstrators			2		2		2


2.2. TREX libraries for software developers and HPC experts

Within the TREX project, state-of-the-art programs for quantum Monte Carlo (QMC) calculations are analysed to identify key algorithms to be then implemented in human-readable, open-source software QMCKI & TREXIO libraries. The libraries are further optimized for future exascale supercomputers by computer scientists of the TREX project.

TREX-Libraries

When entering the field of highly specialized scientific disciplines, software development tends to follow rules shared and agreed upon within that specific scientific community, which, however, are often not reusable by others. The goal of TREX is to reimplement the algorithms in a domain-agnostic way such that HPC experts can easily provide the most efficient implementation for exascale hardware.


Within the TREX project, state-of-the-art programs for quantum Monte Carlo (QMC) calculations are analysed to identify key algorithms to be then implemented in human-readable, open-source software QMCKI & TREXIO libraries. The libraries are further optimized for future exascale supercomputers by computer scientists of the TREX project. The QMC codes within TREX are at different stages of software development but are all algorithmically extremely advanced and uniquely powerful in the landscape of electronic structure methods.



QMCKI

The QMCKI library aims at providing a high-performance implementation of the main kernels of Quantum Monte Carlo methods.

[Read More >](#)



TREXIO

The TREXIO library defines a standard format for storing wave function parameters, together with a C-compatible API such that it can be easily used in any programming language.


[Read More >](#)

Figure 4 TREX Libraries page on the TREX website, available at <https://trex-coe.eu/trex-quantum-chemistry-libraries>

2.2.1. QMCKI Library

Within the TREX project, state-of-the-art programs for quantum Monte Carlo (QMC) calculations are analysed to identify key algorithms to be then implemented in an open-source software library, QMCKI. The library is further optimized for future exascale supercomputers by computer scientists of the TREX project. This library can also be integrated in other quantum chemical codes and, conversely, allow TREX to bring in other codes (and corresponding user communities) which would not otherwise benefit from the exascale transition.

A page dedicated to the QMCKI Library was created on the project website¹, recently updated with information about technical descriptions, partners who contributed to the development and ready to host downloadable and training materials as soon as available. An icon was also custom designed for the library, aligned with the project branding.



QMCKI

The QMCKI library aims at providing a high-performance implementation of the main kernels of Quantum Monte Carlo methods.

Contributors: Anthony Scemama (CNRS), Claudia Filippi (UT), William Jalby (UVSQ), Saverio Moroni (SISSA), Pablo Oliveira Castro (UVSQ), Sandro Sorella (SISSA), Cedric Valensi (UVSQ)

As part of TREX: Vijay Gopal Chilkuri (CNRS), Francois Coppens (UVSQ), Evgeny Posenitskiy (CNRS)

[Code Overview](#)
[Technical Description](#)

The QMCKI library aims at providing a high-performance implementation of the main kernels of Quantum Monte Carlo methods. A first implementation of the library focuses on the definition of the API and the tests, and on a pedagogical presentation of the algorithms. Then, HPC experts can use this initial implementation as a reference to re-write optimized versions of the library with the same API.

Audience

Theoretical chemistry community, quantum simulation of materials community.

[+](#)
[f](#)
[t](#)
[in](#)

Developer





-  Centre National de la Recherche Scientifique (CNRS)
-  University of Twente (UT)
-  SISSA Scuola Internazionale Superiore di Studi Avanzati
-  Max Planck Institute for Solid State Research (MPI)

Figure 5 Preview of the QMCKI dedicated web page

¹ <https://trex-coe.eu/qmckl-library-software-developers-and-hpc-experts-0>

An interview with Anthony Scemama (CNRS/Toulouse) focused on QMCKI was recorded in January 2021 and has been published on the TREX YouTube channel and included in the QMCKI library page².

2.2.2. TREXIO library

The TREXIO library defines a standard format for storing wave function parameters, together with a C-compatible API such that it can be easily used in any programming language. A dedicated webpage provides users with information about TREXIO contributors, current stage and next steps. For this library a custom logo was designed as well.

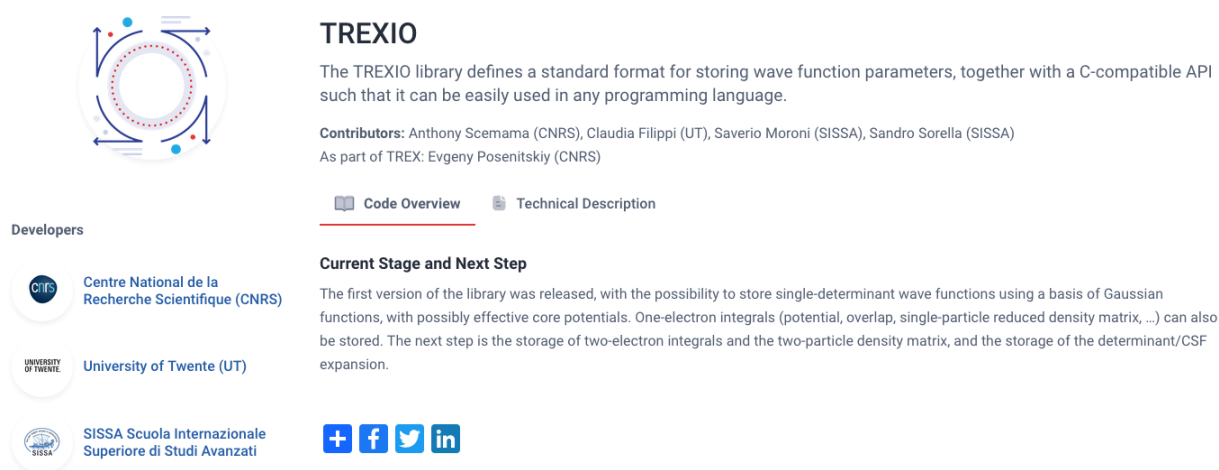


Figure 6 Preview of the TREXIO dedicated web page

For the next period, we foreseen the following dissemination activities specifically related to the TREX libraries:

Activity	Description	M18	M21	M24	M27	M30	M33	M36
Interviews	Interviews with library owners	1		1				
Social media promotion	Post targeting libraries	continuous						
Revamped Library section pages	revamped section on the website introducing libraries incl. technical and training information		1	1	1	1		
Publications	New scientific publications issued about the libraries			1		1		
Third-party events	Promotion of the library with posters and presentations at third party event	1	3	1				

² <https://trex-coe.eu/qmckl-library-software-developers-and-hpc-experts-0>

2.3. TREX Flagship Codes

In addition to the QMCKI and TREXIO libraries, TREX developments target six different codes belonging to the scientific domain of quantum chemistry, not all of them being exclusively QMC codes: **TurboRVB**, **CHAMP**, **QMC=Chem**, **NECI**, **Quantum Package**, and **GammCor**. The promotion of all these codes is at the core of the dissemination strategy of the project.

Custom logos were designed for each of the codes, aligned with the TREX branding and leveraging on pre-existing logos where available.

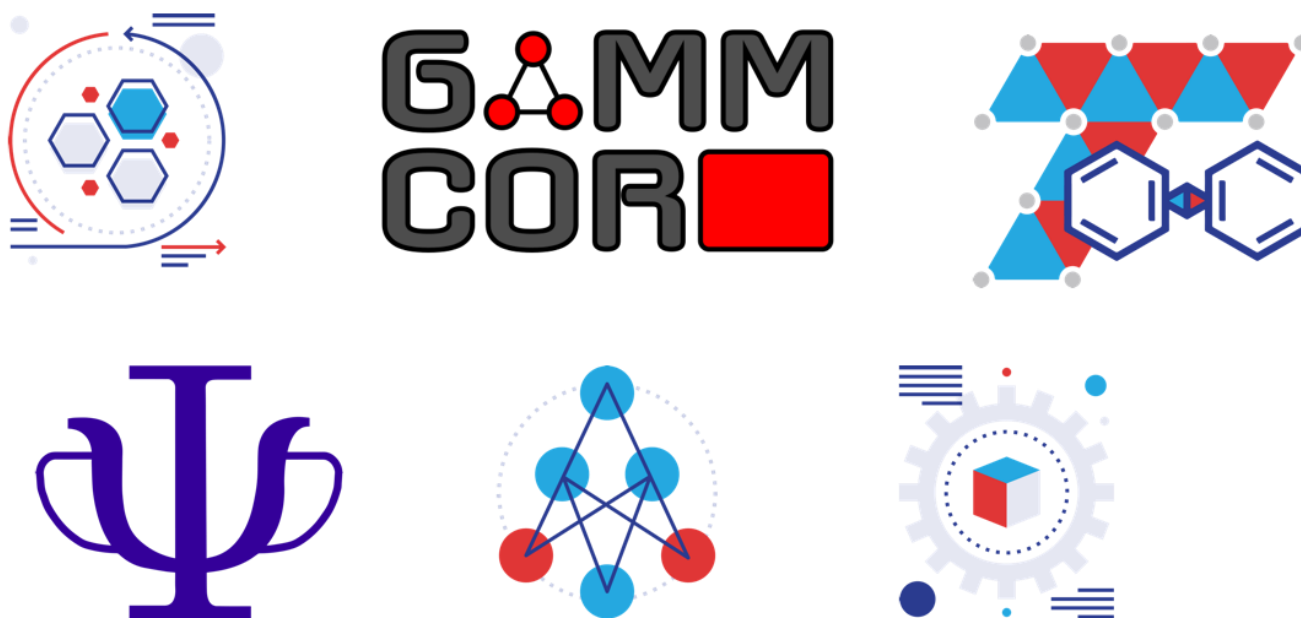


Figure 7 TREX Flagship Code logos

The website section dedicated to the codes was revamped, too, with dedicated pages where to find technical information on each code and ready to host downloadable and training materials as soon as available. To make it easy and intuitive to reach, it was decided to place a link to the code pages within the main “Software menu”. Codes are also part of a continuous social media campaign, with target posts dedicated to each of the codes.



Figure 8 Sample post about the TurboRVB code

Videos are strategic for the dissemination and promotion of the results, therefore interviews have been scheduled with the owners and creators of TREX codes, providing additional authority and increasing the trust that users have on the site. So far 4 video interviews have been realized and distributed via TREX website³ and Youtube channel⁴.



Figure 9 Three of the video interviews realised with TREX partners in this reporting period

The training events planned within WP6 have been disseminated and promoted across TREX social media Twitter and LinkedIn profiles, with custom cards and banners re-shared by HPC social media networks as well as quantum mechanical simulations, such as by Psi-k, the Europe-based, worldwide network of researchers working on the advancement of first-principles computational materials science⁵.

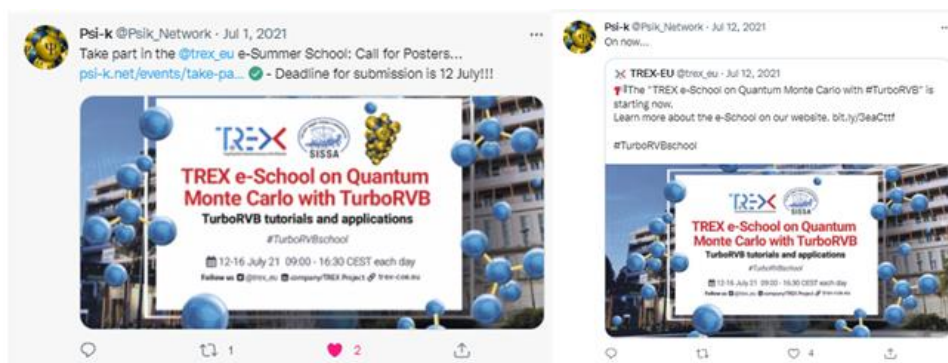


Figure 10 Preview of a PSI-k social media post TREX e-School on TurboRVB

For the next period, we foreseen the following dissemination activities specifically related to the TREX codes:

Table 2 Upcoming dissemination activities specifically related to the TREX codes

Activity	Description	M18	M21	M24	M27	M30	M33	M36
Interviews	Interviews with code owners		1	1	1	1		
Social media promotion	Post targeting codes	continuous						
Technical and training	Technical and training materials added to the code				X	X	X	

³ <https://www.trex-coe.eu/our-videos>

⁴ <https://www.youtube.com/channel/UCGkQzeUW6077jLpUEtm2RDA/videos>

⁵ <https://psi-k.net/>

Activity	Description	M18	M21	M24	M27	M30	M33	M36
materials	pages and disseminated							
Publications	New scientific publications issued about the codes			1		1		1
Third party events	Promotion of the codes with posters and presentations at third party event	1	3	2		1		
Code webinars	Organisation of TREX code webinars		1	1	1	1	1	1

3. TREX community building: Stakeholder engagement up to M18

One of the key pillars of TREX is an outreach programme to the relevant developers' and users' communities to foster the use of the developed HPC codes as well as engage and forge a new generation of highly-skilled computational scientists. The current COVID-19 situation has disrupted the delivery of physical events and participation at events during the first period of the project. Partners have intensified online meetings and have turned physical events into online ones, ensuring the same engagement level and meeting the expected KPIs.

Several virtual events have been organised by WP6, which are highlighted in Sections 3.1 and 3.2. Moreover, TREX partners took part in several events organized in collaboration with FocusCoE, EU CoEs, and other relevant organisations in the field, which will be described in Section 3.3. WP7 ensured that each partner had corresponding support such as live social media visibility during the event, publication of the event news on the website and pre-event promotion.

While smooth operations and regular flow of online events will continue as long as the COVID crisis persists, physical events have recently started again with the Hackathon II and the TREX meeting organised in Versailles from 28 February to 3 March 2022.

3.1. TREX Workshops and Schools

TREX training activities (WP6) aim to increase the expertise of the wider community not only in the scientific application and HPC usage of TREX software but also more generally in HPC, democratizing the use of upcoming computational (pre)exascale resources.

3.1.1. TREX e-School on quantum Monte Carlo with TurboRVB

The TREX e-School on QMC with TurboRVB was jointly organised by TREX, together with the Psi-k network⁶ and the International School for Advanced Studies (SISSA)⁷, from 12 to 16 July 2021.

⁶ <https://psi-k.net/>

⁷ <https://www.sissa.it/>



Figure 11 Official event banner for the TREX e-School on QMC with TurboRVB, 12-16 July 2021 - Online event

WP7 assisted the event organisers in setting up the event's platform, the registration process (including an automatic referral form for their applicant supervisors, which was used to select the hands-on participants), and creation of the TREX Zoom account, where the event was hosted. This event also offered its attendees the opportunity to present their latest results and contributions in the field by submitting a poster⁸. The best poster winner received as prize a printed copy of the book "Quantum Monte Carlo Approaches for Correlated Systems"⁹ written by Sandro Sorella and Federico Becca¹⁰. The event received 89 valid applications from Master and PhD students, postdocs, researchers, and HPC experts, of which 66 (from 33 countries and 4 continents) were admitted to the public plenary lectures and 24 were selected to follow the hands-on tutorials in the afternoons. More than 50 students connected each day to follow the lectures.

Post-event materials have been published on the event page, including recordings of the public sessions and presentations¹¹, participants list¹² and a post-event report¹³.

⁸ <https://trex-coe.eu/trex-e-school-quantum-monte-carlo-turborvb-2021-posters-0>

⁹ https://www.amazon.it/Quantum-Monte-Approaches-Correlated-Systems/dp/1107129931/ref=sr_1_1?crd=330R3KZIOZEJE&dchild=1&keywords=quantum+monte+carlo+approaches+f+or+correlated+systems&qid=1631543466&sr=8-1

¹⁰ <https://www.trex-coe.eu/events/trex-e-school-quantum-monte-carlo-turborvb>

¹¹ <https://trex-coe.eu/trex-e-school-quantum-monte-carlo-turborvb-recordings-and-presentations>

¹² <https://trex-coe.eu/sites/default/files/TREX%20e-School%20QMC%20with%20TurboRVB%20-%20July%202021/TREX%20e-School%202021%20-%20Participants%20List.pdf>

¹³ <https://trex-coe.eu/new-generation-hpc-developers-using-quantum-monte-carlo-qmc-methods-growing>

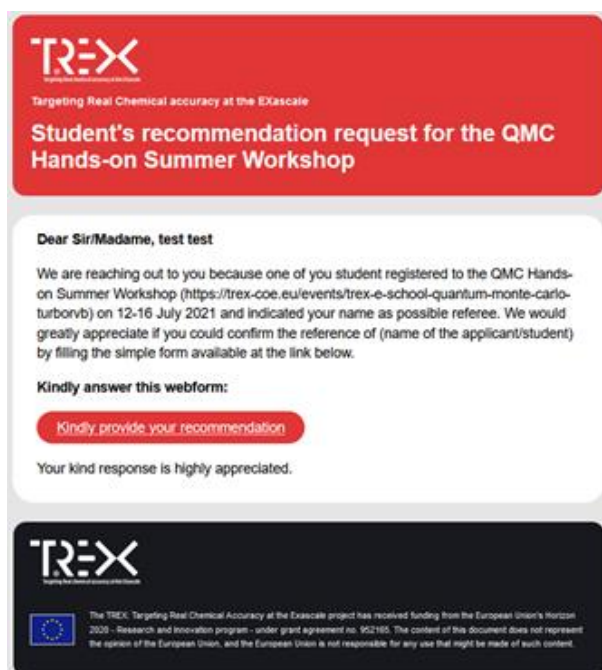


Figure 8 – TREX e-School – Automated Student's referral request

This event has received positive feedback from the attendees. Some of the feedback received are included in the post event report available on the event page¹⁴. A light satisfaction survey was circulated after the school.

TurboRVBSchool - Satisfaction Survey	Average Rating (0-5)
Rate the organisation, logistics and videoconferencing tools used	4,7
How would you rate the programme?	4,6

Table 3 TurboRVBSchool – Outcomes of the satisfaction Survey

Testimonials¹⁵ were gathered from the attendees during the plenary sessions and the hands-on tutorials, showcasing their feedback regarding the event.

¹⁴ <https://trex-coe.eu/new-generation-hpc-developers-using-quantum-monte-carlo-qmc-methods-growing>

¹⁵ <https://trex-coe.eu/testimonials>



Figure 12 Testimonials from the attendees of TREX e-School on QMC with TurboRVB

At the moment of writing, 39 members of the SISSA github TurboRVB repository have downloaded the code and 20 people out of this group have recently worked with TurboRVB.

3.1.1. TREX session at the virtual PRACE booth at ISC 2021¹⁶ (24 Jun – 2 Jul 2021, Virtual)

The ISC conference is the Europe's leading digital conference in the field of computer science, attended by over 2000 international attendees and 84 exhibitors, for high performance computing, machine learning (ML), and high performance data analytics (HPDA) this year. On 2 July 2021, TREX participated in the PRACE virtual booth¹⁷ at the ISC Conference, organised from 24 June to 2 July 2021 with the support of the FocusCoE. Anthony Scemama (CNRS, Toulouse) and Pablo de Oliveira Castro, Cédric Valensi, and William Jalby (Université de Versailles St-Quentin-en-Yvelines) presented the progress achieved with the TREX codes and libraries. The presentation showcased TREX innovative view of HPC usage applied to quantum Monte Carlo simulations to over 30 HPC participants.

The session at the PRACE virtual booth required an online registration that was set-up by the WP7 Trust-IT team on the TREX website¹⁸. Promotion before, during, and after the event was also ensured.

¹⁶ <https://www.trex-coe.eu/events/isc-2021>

¹⁷ <https://prace-ri.eu/event/praceisc-2021/>

¹⁸ <https://trex-coe.eu/events/isc-2021>



Figure 13 Event banner for the PRACE booth at ISC21, 2 July 2021, Online event

3.2. Training events: TREX Hackathons

TREX structured training and educational activities (lead by WP6) cover different facets from technical support to the end-users of the TREX software, hands-on training for code users from academia and industry, and hands-on workshops to train code developers.

Two TREX Hackathons were organised so far as detailed in the following paragraphs.

3.2.1. TREX Build-systems Hackathon, 8-12 November 2021

This first TREX Hackathon was a multi-day virtual event¹⁹ targeting students, engineers, and researchers developing HPC open-source software. The goal was to help these code developers to better understand how to use build-systems tools to improve the portability of their applications. Making HPC software easy to install on multiple supercomputers or different architectures is a difficult task since many systems have different compilers, libraries, system commands etc. This task can be helped by tools like CMake²⁰ and GNU Autotools²¹, which were supported for this Hackathon. Well-done configuration scripts facilitate the packaging of the software, and presentations were also given to propose different packaging possibilities to distribute the software.

¹⁹ <https://www.trex-coe.eu/events/trex-build-system-hackathon-8-12-nov-2021>

²⁰ <https://cmake.org/>

²¹ <https://www.gnu.org/software/autoconf/>



Figure 14 TREX Build-systems Hackathon promotional banner

45 participants from 21 countries attended the online event. A group of nine (9) mentors²² was created to support code developers in better understanding how to use these build systems to improve the portability of their applications using TREX codes. In support to WP6, the WP7 team created the official event page on the TREX website, hosting all the post-event materials such as the plenary presentations²³ and video recordings of the sessions²⁴.

3.2.2. TREX Hackathon II, 28 February-4 March, 2022

The subsequent TREX Hackathon “TREX Hackathon II with TREX event at UVSQ”²⁵ has been organised in a physical format from 28 February to 4 March 2022 at the premise of the Université de Versailles-Saint-Quentin-en-Yvelines (UVSQ)²⁶. During the event, the consortium took advantage of a first face-to-face (F2F) meeting including all TREX participants, which followed the Hackathon on the 3rd and 4th days of the event (2-3 March).



Figure 15 Pictures taken at the TREX Hackathon II in Versailles

²² <https://www.trex-coe.eu/events/trex-build-system-hackathon-8-12-nov-2021>

²³ <https://www.trex-coe.eu/trex-build-systems-hackathon-presentations>

²⁴ <https://www.youtube.com/watch?v=5ikM3deCRPA&list=PLtNjYPIYe2t2REVPUbmWY36DOoTjwEGUa>

²⁵ <https://www.trex-coe.eu/events/trex-hackathon-ii-trex-event-uvsq>

²⁶ <https://www.trex-coe.eu/events/trex-hackathon-ii-trex-event-uvsq>

3.3. TREX events: some figures

For the TREX Build-systems Hackathon (8-12 November 2021) and the TREX e-School on quantum Monte Carlo with TurboRVB (12 to 16 July 2021), online registration was organised on the TREX website. Online registration was also set-up for the session organised at the PRACE virtual booth at ISC2021 (2 Jul 2021). Looking at the overall community engaged via the TREX website for these events, a total of 174 live attendees participated in these events coming from 40 different countries around the world.

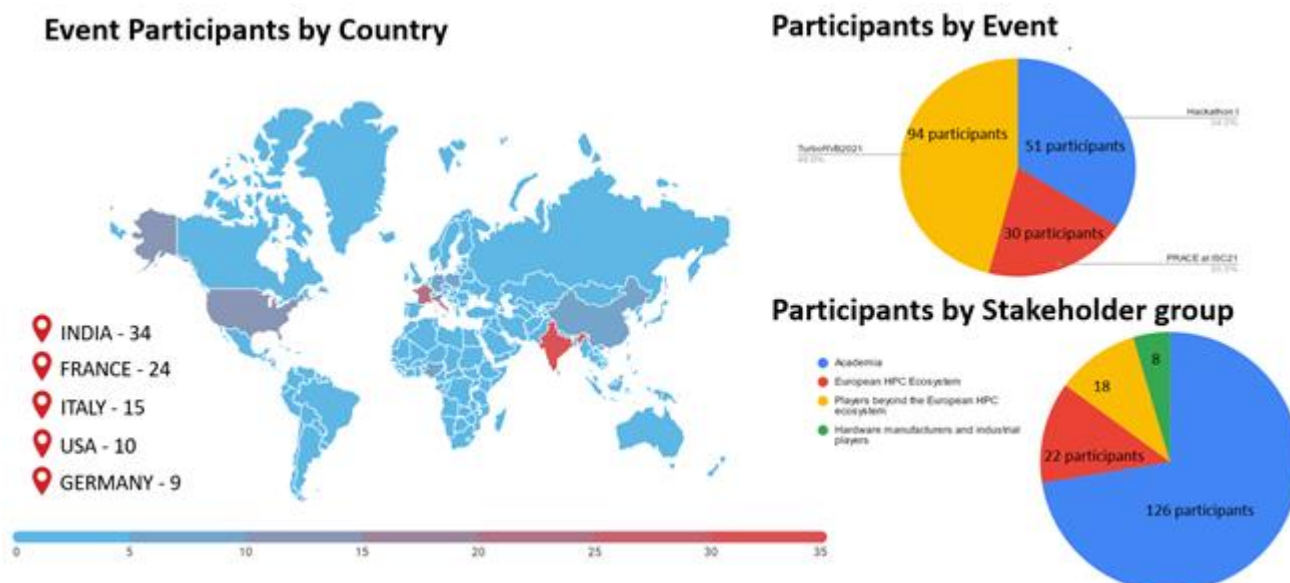


Figure 11 – TREX participation at TREX 2021 online events (TREX Build-systems Hackathon, TREX e-School on quantum Monte Carlo with TurboRVB and Session at ISC2021) by country and stakeholder group

3.4. Other events

Partners from the Consortium participated in 20 events at national, European, and international level, including events within the EU HPC ecosystem organized with/by the HPC Centre of Excellence Council (HPC3)²⁷, FocusCoE, EuroCC National Competence Centers, and other CoEs; training events on HPC advancements or domain-specific topics targeting industrial and academic audience including students, postdocs, and researchers, and industrial players.

Participation spans virtual and physical presentations, panel debates, workshops, and tutorials for focused and effective communication, dissemination, and engagement outcomes, with live reporting via Twitter and LinkedIn posts.

An “Event Tracker” is being maintained in the Microsoft Team collaboration platform to keep tidily track of the participation of TREX partner at relevant third-party events.

²⁷ <https://www.hpccoe.eu/hpc-coe-council/>

Count	Event	Date	Participating Part Venue	Link	TREX URL	Target participants	No. of participants
1	HPC3 Council (June 2020)	giu-20	UT				
2	The importance of being H.P.C. Earnest (CECAM webinar series)	18-giu-20	Claudia Filippi (U Online)	https://www.cecama.org/webinar-details/nicola-marzari-claudia-filippi-anthony-scemama-giulia-galli		General computational	
3	Instructor training workshop for HPC CoEs	nov-20	UVSQ				
4	FocusCoE Centres of Excellence Webinar: Interaction with Industry and SME	27-nov-20	Megware, CNRS Online	https://www.hpccoe.eu/index.php/about/	https://www.trex-coe.eu/events/focuscoe-centres-excellence-webinar-interaction-industry-and-sme		
5	Webinar on the interaction with industries and SMEs	dic-20	Megware, CNRS				
6	Tuning Workshop, Vi-HPS	7-11 Dec 2020	Cedric Valensi (U Online)	https://csc.uni-frankfurt.de/wiki/doku.php?id=public-events#vihps_tuning_workshopdecember_2020	https://www.trex-coe.eu/events/tuning-workshop-vi-hps		
7	Luchon Winter School - TREX Tutorials in Quantum Monte Carlo (QMC)	25 Jan - 8 Feb 2021	Claudia Filippi (U Online)	https://www.irsamc.upstlse.fr/ttc/	https://www.trex-coe.eu/events/luchon-winter-school	International TCCM ma	23
8	3rd EMMC International Workshop	2-4 Mar 2021	Fabio Affinito (CI Online)	https://emmc.eu/emmc-2021/	https://www.trex-coe.eu/events/3rd-emmc-international-workshop-2021	speaker - please supply	speaker - please suppl
9	CoEs Co-Design Workshop	12-mar-21	Anthony Sceman Online		https://trex-coe.eu/events/coes-co-design-workshop	Members of CoEs	speaker - please suppl
10	Helmholtz GPU Hackathon 2021 - Digital Event	15-24 Mar 2021	Anthony Sceman Online	https://bit.ly/2XdCYtz	https://www.trex-coe.eu/events/helmholtz-gpu-hackathon-2021-digital-event	all organisations interes	Dirk - please supply th

Figure 16 Preview of the event tracker on TREX Microsoft Teams collaborative platform

All the events are listed in ANNEX II .

Outcomes and impacts of the most relevant events are described below.

3.4.1. Luchon Winter School of the Erasmus Mundus TCCM program²⁸ (first event on 25 January - 8 February 2021)

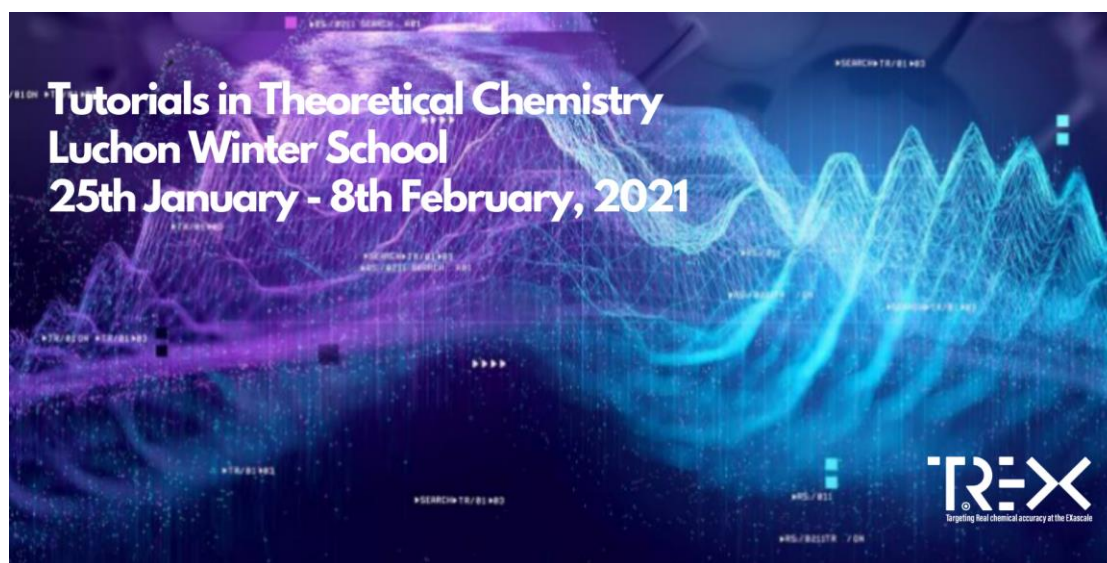


Figure 12: Event banner for the Luchon School of the Erasmus Mundus TCCM program, 25 Jan-8 Feb 2021, Online event

TREX organizes a yearly satellite hands-on event as a one day on quantum Monte Carlo methods in chemistry at the Luchon Winter European School. The school is organized by the European Erasmus Mundus Joint Master Degree program on Theoretical Chemistry and Computational Modelling (TCCM), an initiative of 25 European institutions from 6 different EU countries to prepare experts in the use and development of computational techniques in molecular science. The School focuses on training the Master students in the computer implementation of methods in quantum chemistry, also featuring the TREX project. The first satellite TREX event took place between 25 January and 8

²⁸ <https://trex-coe.eu/events/luchon-winter-school>

February 2021 (online). With over 25 master's students and 1st year PhD students who attended the event, TREX partners Claudia Filippi (UT) and Anthony Scemama (CNRS/Toulouse) participated in the event by teaching the basic concepts of quantum Monte Carlo (QMC) methods and explaining how to write a simple QMC program.

During this event, we had the opportunity to get testimonials from the attendees, available at the dedicated page on the TREX website²⁹.



Testimonial: Luchon Winter School of the Erasmus Mundus

During the Luchon Winter School of the Erasmus Mundus training event, held from 25th of January to 8th of February 2021, Claudia Filippi (TREX coordinator) and Anthony Scemama (scientific partner) from TREX participated by teaching to introduce the basic concepts of Quantum Monte Carlo (QMC) methods and explain how to write a simple

Figure 13– Attendees' Testimonials from the Luchon Winter TCCM European School

3.4.2. CECAM2021: Recent developments in quantum Monte Carlo³⁰ (21-22 Oct 2021, Italy)



Figure 14: Event banner for the CECAM Workshop, 21-22 October 2021, Rome (IT)

CECAM (Centre Européen de Calcul Atomique et Moléculaire) promotes fundamental research on advanced computational methods and their application to important problems in frontier areas of science and technology. Fabio Affinito, TREX partner leading the specialistic support team at CINECA, was one of the organizers of the meeting and also presented a poster showcasing the "TREX: Targeting Real Chemical accuracy at Exascale³¹". Furthermore, the following talks were given by TREX partners:

²⁹ <https://www.trex-coe.eu/testimonials>

³⁰ <https://www.trex-coe.eu/events/cecam-2021-workshop-recent-developments-quantum-monte-carlo>

³¹ <https://www.cecam.org/workshop-details/1050>

- 05. Phase diagram of high-pressure hydrogen including nuclear quantum effects³² - Michele Casula, CNRS
- 08. Variational principles and excited states in quantum Monte Carlo³³ - Claudia Filippi, University of Twente and TREX Project Coordinator
- 16. The phase diagram of the Hubbard model by Variational Auxiliary-Field QMC³⁴ - Sandro Sorella, SISSA

3.5. Upcoming Events

As we entered 2022, the TREX team is taking the opportunity to hold the training and dissemination activities as physical events. Below is a preliminary list of upcoming 3rd-party training, HPC, and domain-specific conferences that TREX partners are planning to attend.

Table 1 – Upcoming 3rd-party HPC and domain-specific events

Event	Date	Location	Type
EuroHPC Summit week 2022/PRACEdays22 (EHPCSW 2022)	22-24 Mar 2022	Paris, France	3rd-party event
Girls Day University Twente	7 April 2022	Enschede, The Netherlands	3rd-party event (co-sponsored by TREX)
ISC2022	29 May – 2 Jun 2022	Hamburg, Germany	3rd-party event
10 th OpenMolcas Developers Workshop	8-10 Jun 2022	Uppsala, Sweden	3rd-party event (co-sponsored by TREX)
HiPEAC 2022	20-22 Jun 2022	Budapest, Hungary	3rd-party event
PASC2022	27-29 Jun 2022	Basel, Switzerland	3rd-party event
TERATEC Forum 2022	14-15 Jul 2022	Paris, France	3rd-party event
International Summer School on Electronic Structure Theory and Materials Design	14-19 Aug 2022	Helsingør, Denmark	3rd-party event
Psi-k Conference 2022	22-25 Aug 2022	Lausanne, Switzerland	3rd-party event
Luchon Winter School	Jan 2023	Luchon, France	3rd-party event

3.6. Outreach and promotion of upcoming TREX training activities

For all the upcoming TREX training events, dissemination and promotion will be ensured by WP7. This includes support in managing online pages and registration, poster sessions, information and social media campaigns and collateral activities as well as support for on-site logistics when needed for physical events.

³² <https://www.cecami.org/workshop-details/1050>

³³ <https://www.cecami.org/workshop-details/1050>

³⁴ <https://www.cecami.org/workshop-details/1050>

Upcoming training events include:

Period	Title	Location	Organising partners
March - December 2022	TREX Hackathon III 2022 (delayed due to the reschedule of the installation of Leonardo supercomputer)	Bologna, Italy	CINECA/UVSQ
	QMC Hands-on Summer Workshop	Bratislava, Slovakia	SAV
	TREX e-school on Quantum Monte Carlo with TurboRVB #2	Trieste, Italy	SISSA
	CESTC 2022 QMC satellite	Balaton, Hungary	TREX, A.S., C.F., I.S.
	Workshop on TREX platform & ML	Lodz, Poland	TUL
	School: TREX SW & ML & AiiDA	Trieste, Italy or Lausanne, Switzerland	UT
January-September 2023	Code Developer Workshop	Bratislava, Slovakia	SAV
	Hackathon # IV - Final code optimization	TBD	TBD

4. TREX and HPC Ecosystem

Since Summer 2020, TREX joined the HPC Center of Excellence Council which was established to coordinate common CoE strategies and joint actions as well as ensure support for application development within the HPC landscape shaped by EuroHPC. The TREX coordinator (UT) and/or her deputy (CNRS/Toulouse) attends the monthly meetings of the Council which have been found to be a very useful platform to interact with other CoEs, learn about European initiatives where TREX can contribute, and provide concrete feedback to the EC via the HPC3 Management Board.

4.1. Participation into FocusCOE activities

TREX team has been actively synergising in the regular initiatives promoted by the Coordinated Support Action (CSA) FocusCoE, funded to aid CoEs to fulfil their role in synergy within the HPC ecosystem. Several TREX partners are participating in the discussion for the main transversal actions led by the FocusCoE such as industrial outreach, training, and dissemination.

Moreover, TREX partners participated in several HPC events as attendees or by giving presentations or joining panel discussions, where TREX goals, software strategies, and expected outputs were presented to the representatives of all CoEs. Below is the list of events attended in the past year.

Table 1 – TREX participation in FocusCoE events

Event	Date
Participation (UVSQ) to Instructor Training Workshop	November 2020
Participation (CNRS/Paris, Megware) in the Webinar on the interaction with industries and SMEs	December 2020
Participation (CINECA, CNRS/Toulouse) in Co-design Workshop for CoEs	March 2021
Participation (CNRS/Toulouse, USVQ) by joining the dedicated virtual PRACE booth at ISC 2021	July 2021
Participation (UT, CNRS/Toulouse) in NCC-CoE meeting on First-Principle Simulations in Chemistry and Materials Science	July 2021
Participation (UVSQ) in NCC-CoE meeting on Code Optimization	November 2021

4.2. Collaboration with other HPC CoEs

In addition to the regular exchanges with other CoEs via HPC3, High Performance Community Computing Cluster³⁵ and FocusCoE, TREX has established contacts and, in some cases, strong collaborations with selected CoEs as described below.



MaX CoE: TREX focuses on high-accuracy quantum mechanical stochastic simulations and, as such, is complementary to MaX in methodology, actual software, and typology of quantum problems usually addressed: TREX approaches are algorithmically totally distinct to the ones adopted in MaX and our flagship codes produce generally different kind of predictions of quantum chemical and material properties that are typically more accurate and more computationally demanding. In this complementarity resides also the synergy between MaX and TREX. In fact, TREX is currently capitalizing on and enhancing one infrastructural initiative of Max, having adopted the AiiDA Materials Informatics Framework developed within MaX for workflow management, data storage, persistence, and provenance.

Joint events and/or meetings were organised in Oct and July 2020, October and November 2021:

- Key developers from the AiiDA team (Dr. Giovanni Pizzi and Dr. Sebastiaan Huber) were asked to present the main features of AiiDA and give a tutorial at the **TREX Kickoff Meeting of WP4** (October 2020).
- Several TREX members (SISSA, CNRS/Toulouse, UT, Megware) participated to the **AiiDA Virtual Tutorial Week** on running and writing workflows with AiiDA (July 2021).
- Because of TREX interest and expertise in interoperability, TREX representative (CNRS/Toulouse) was invited to chair a session at the International Workshop on **“Ontologies for materials-databases interoperability”** (October 2021) co-organized by Dr. Giovanni Pizzi (AiiDA/EPFL/NCCR MARVEL).

³⁵ <https://rcic.uci.edu/hpc3/#>

- Dr. Leopold Talirz (AiiDA/Materials Cloud/EPFL) was invited to give a presentation on Software Packaging at the **TREX Build-systems Hackathon** (November 2021). Generating a container for TREX software is part of Task T7.3 “TREX outreach strategy and synergies with related HPC initiatives” (**WP7**).

Nicola Marzari is member of TREX Advisory Board. His profile is online at the page Advisory Board dedicated page:



The TREX Expert Advisory Board (EAB) has been established to assist the TREX project, which will play an important role in supporting the CoE in its scientific directions, as well as in legacy and sustainability strategy. The EAB is composed of recognised experts in the HPC ecosystem, from academia, industry and relevant policy bodies. They will follow the development of TREX and provide advice and feedback on TREX exploitation and sustainability strategies.

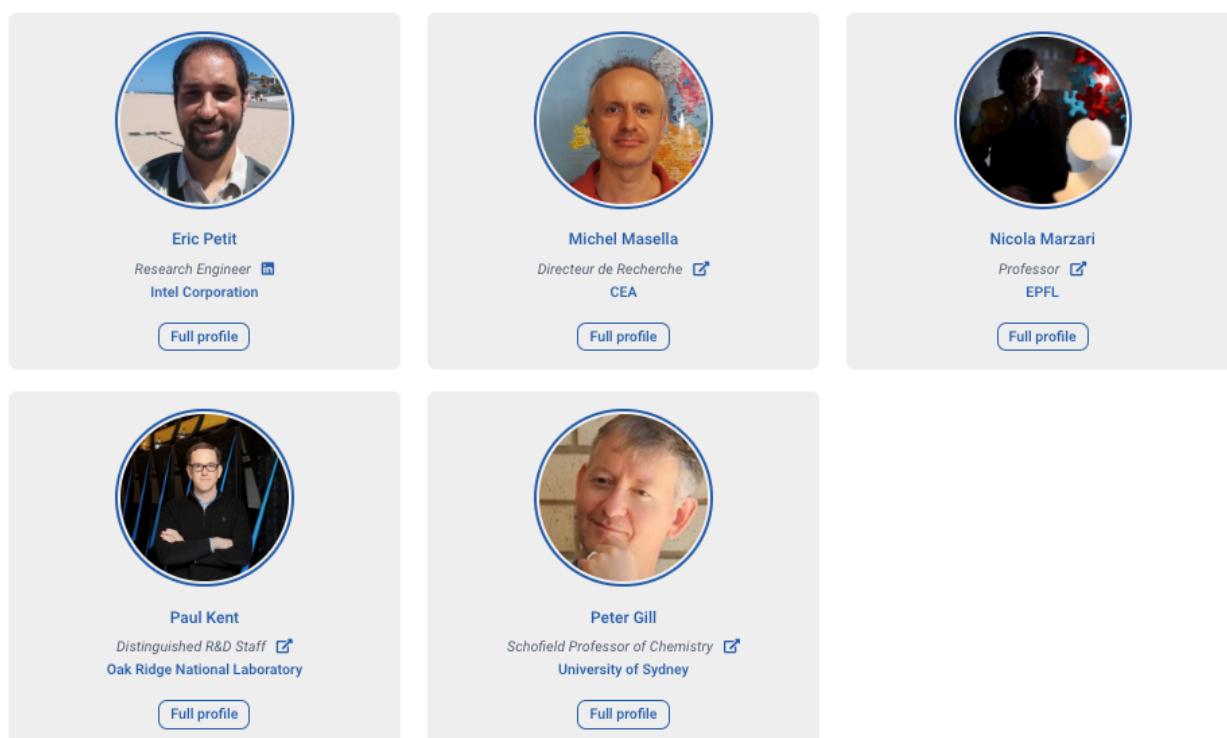


Figure 16 TREX Expert Advisory Board page



POP2CoE: We are connected to the **Performance Optimization and Production CoE** (POP2) through our partner UVSQ. POP aims at offering a portfolio of services designed to help users to optimise parallel software and understand performance issues. Among these services, there is an important focus on **application performance assessment**, through a set of performance metrics that will be used during the design and optimisation of TREX codes and libraries. Within PoP, UVSQ has been mainly involved in single-core and single-node performance analysis using **MAQAO** and, in the past year, the acquired experience and knowledge have been leveraged to analyse and optimize **TREX flagship codes** and the **QMckI library**.



NOMAD. Contacts through individual NOMAD members and invitations to present TREX software outputs took place in April 2021 and June 2021:

- TREX presentation (CNRS/Toulouse) on “Library development within TREX” at **Gruneis’ Group, Vienna University of Technology**, Austria (April 2021).
- TREX presentation (UT) on “Software strategy and goals of TREX CoE” at the **10th ABINIT International Developer Workshop** (June 2021)
- TREX tutorial lecture (UT) on “Quantum Monte Carlo” was organised at the International Summer School on Electronic Structure Theory and Materials Design, by the **Computational Atomic-scale Materials Design** Section at the Technical University of Denmark (August 2022).

Gruneis’ Group (NOMAD) expressed their interest in adopting a common file format and using the Input/Output TREXIO library (WP2).

4.3. Future Engagement with European HPC CoEs

Together with the Max Planck Computing and Data Facility and the Barcelona Supercomputing Center, the CoEs NOMAD, MaX, BioExcel, and TREX are organizing a CECAM E-CAM Workshop on “Codesign for HPC in the Materials and related Sciences”, which is now planned for October 2022.

Additional outreach activities are foreseen with other European HPC CoE for the months to come as presented in the table below.

Table 4 Upcoming engagement activities with European HPCs

Activity	Description	M18	M21	M24	M27	M30	M33	M36
Interviews	Interviews with Nicola Marzari				1			
Flyer	TREX HPC Impact Brochure for FocusCOE		1					
Joint events	Joint participation to third party events			1				
Webpage	TREX in the HPC ecosystem page			1				

5. Communication activities and KPIs

5.1. Website

TREX website is the central hub for all the communication and dissemination for the project and is the main reference for all the assets and services. The initial landing page was created on M1 of the project, while the full development of the website was completed at the beginning of March 2021 (M6 - see D7.3).

The website not only has an intuitive design and modern architecture but also includes many features with user experience in mind, helping the users to quickly and easily navigate the site and learn more

about the TREX project, its assets, and services (e.g. software, demonstrators, training, and events). As of today, the information architecture of the TREX website is the one shown below:

- About
 - Partners
 - People
 - Communication Kit
 - Our videos
 - TREX Expert Advisory Board
 - Testimonials
- Open Positions
- Software
 - TREX codes
 - TREX libraries
- Demonstrators
 - Energy
 - Graphene
 - Magnetism
 - Water
- Training
- Events
 - Workshops and Schools
 - Hackathons
 - Webinars
 - HPC & other events
- News
- Publications

At the time of writing, the website registers 9300+ users (with 82.2% improvement), 13.9K sessions (with 79.3% improvement), 35.8K pageviews (76.05% improvement).

The geographical breakdown of the users visiting the TREX website is displayed in the figure below. Italy, France, and the Netherlands are the European countries where most of the TREX users are based. The website is monitored through Google Analytics and the performance is displayed via a Google Data Studio dashboard, which is available on the website's Communications Kit – TREX Communication trends³⁶.

³⁶ Communication Kit | TREX (trex-coe.eu)

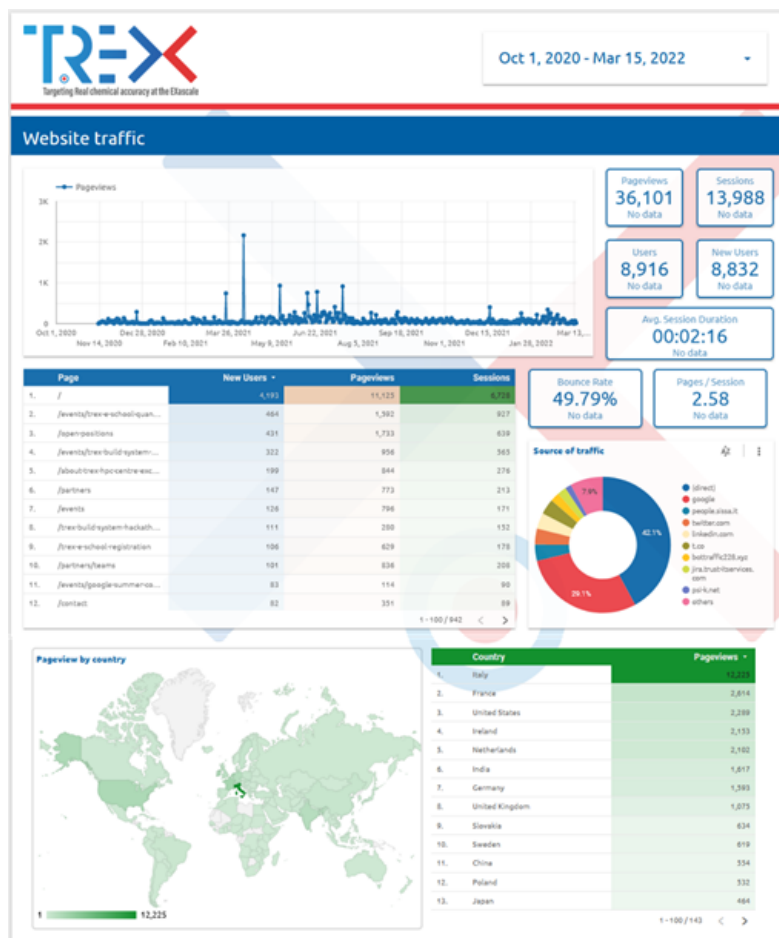


Figure 17 Overall Website performance from October 2020 to mid-March 2022 (M1-M18)

5.2.Social Media

TREX social media channels (Twitter and LinkedIn) have been an essential element in the creation of a growing online community of the TREX project, being catered to and ensured by WP7. In March 2022, the TREX Twitter profile (@trex_eu) counts 209 followers and 165 tweets, and the LinkedIn page (in/company/ trex-eu) counts 341 followers and 169 posts, while the LinkedIn profile counts 406 connections.

Below are some of the examples of the topmost tweets, mentions, and retweets of the TREX project, which demonstrate the collaborations and initiatives through events and website.



Figure 18 TREX Social Media engagement dashboard monitoring (M1-M18)

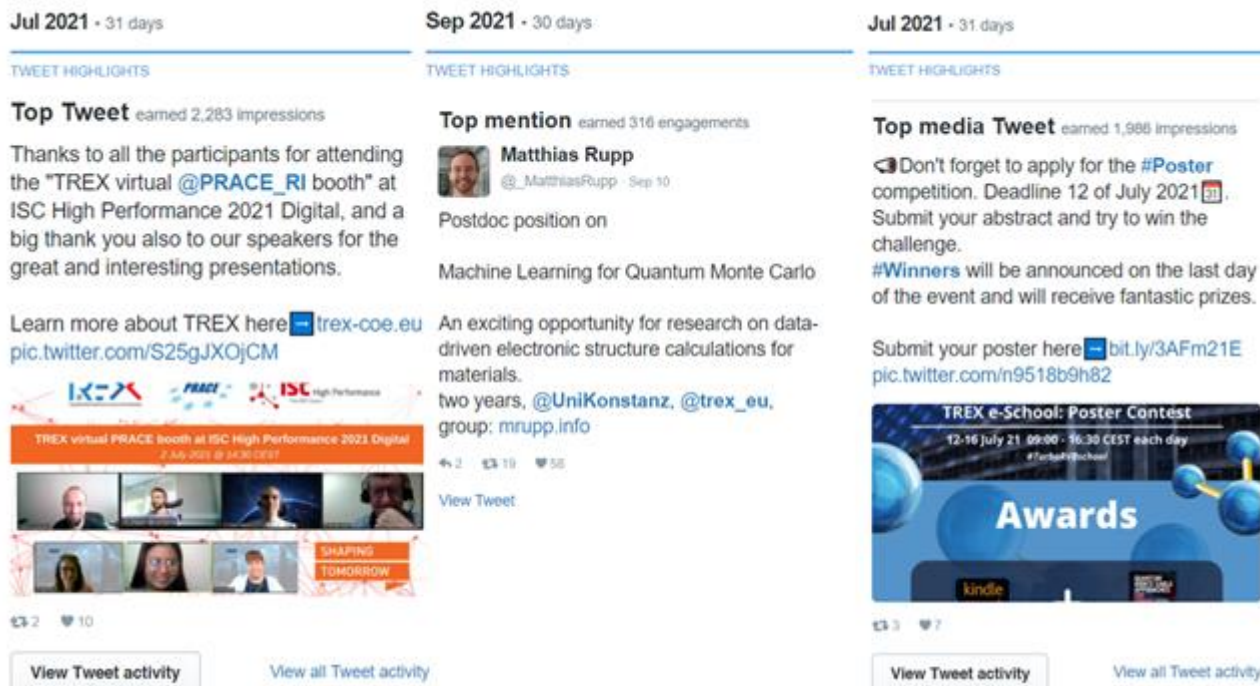


Figure 19 Examples of TREX tweets and mentions

The TREX team leverages the LinkedIn channel to provide professional networking opportunities to its events and open positions. The majority of the social media audiences are from the research community (29%) followed by the education stakeholder group (16.3%).

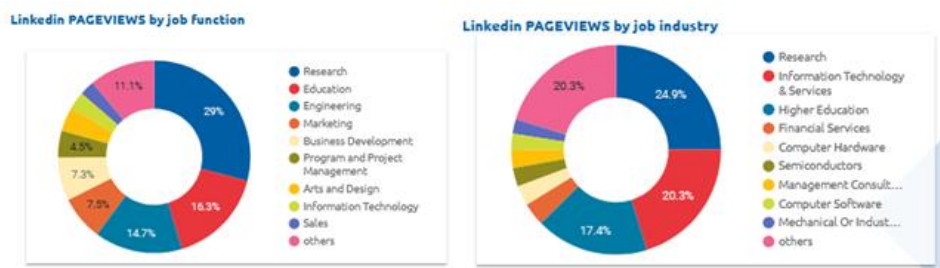


Figure 20 Social media community by job function and industry

5.3. TREX papers and publications

At the moment of writing, there are 15 peer-reviewed articles and 6 reports in the TREX Zenodo community³⁷. The complete list of the TREX publications is also available in ANNEX III.

Publications

Want to learn more about TREX? On this page, you can find our archive of informative publication materials: reports, deliverables, presentations and articles from experts within the TREX community speaking about various TREX related topics. All the public materials published by TREX partners are available on the TREX Zenodo Community: [Zenodo](#)

- Any - Articles Deliverables Presentations Reports

ARTICLES
15
FEB
2022

Dispersion Interactions between Molecules in and out of Equilibrium Geometry: Visualization and Analysis

The Journal of Physical Chemistry A 2022, 126, 7, 1312–1319
Piotr H. Kowalski, Agnieszka Krzemińska, Katarzyna Pernał, Ewa Pastorczak
DOI <https://doi.org/10.1021/acs.jpca.2c00004>

ARTICLES
28
DEC
2021

Calculation of Rényi entropy in realistic quantum systems

Cornell University
Michele Casula, Miha Srdinšek, Rodolphe Vuilleumier
ARXIV <https://arxiv.org/abs/2112.14199>

ARTICLES
20
DEC
2021

Energy Derivatives in Real-Space Diffusion Monte Carlo

Journal of Chemical Theory Computation
Claudia Filippi, Jesse van Rhijn, Stefania De Palo, Saverio Moroni
DOI <https://doi.org/10.1021/acs.jctc.1c00496>

Figure 21 Publication section on the website

³⁷ <https://zenodo.org/communities/trex>

TREX news and events have been promoted by several 3rd party media such as HPCwire³⁸, European Commission’s EU research results³⁹, HPC blogger⁴⁰ providing visibility to a wide range of stakeholders from the academia and research community.



Figure 22 Example of TREX promotion with the 3rd party media

Three newsletters were released in this reporting period to inform the online community of the project activities and developments. These are distributed to a database of more than 100 individuals.

Table 5 TREX newsletters overview

Newsletter	3 newsletter releases (quarterly)
Subscribers	101 subscribers
Open rate	47.0% with a total of 140 opened
Click-through rate	12.1% with a total of 36 clicked
Click-to-open rate	25.7 (as of 4 Mar 2022)

Note: The average email open rate is between 15-25%. The average click-through rate is about 2.5%. The average click-to-open rate is between 20-30%

³⁸ <https://www.hpcwire.com/off-the-wire/trex-organizing-e-summer-school-on-quantum-monte-carlo-with-turborvb/>

³⁹ <https://cordis.europa.eu/article/id/422583-providing-the-research-community-with-unique-exascale-computational-power-instruments-to-push>

⁴⁰ <https://www.ch.imperial.ac.uk/rzepa/blog/?p=24543>

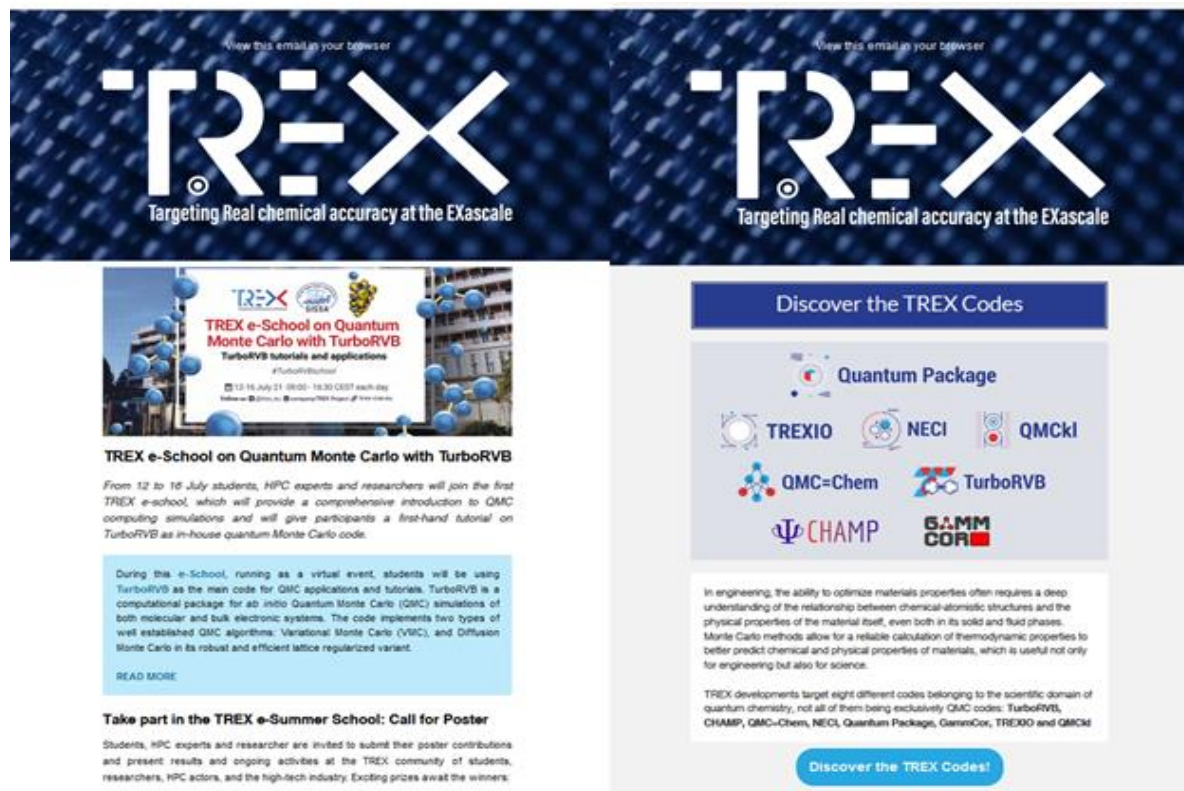


Figure 23 Example of TREX newsletters

5.4. TREX dissemination materials

During this reporting period, WP7 designed the project pop-up banner and the project overview flyer, which were used for the first time during the TREX Hackathon in Versailles.

WP7 is currently contributing to an HPC Impact brochure lead by FocusCoE.

TREX
Targeting Real Chemical Accuracy at the Exascale

Centre of Excellence in HPC for Quantum Chemistry

Targeting Real Chemical Accuracy at the Exascale

UNIVERSITY OF TWENTE, CNRS, SISSA, CHECA, UNIVERSITY OF VERSAILLES, MEGWARE, SAV, TRUST-IT SERVICES

Contact
@trex_eu | /company/trex-eu | t.ly/1Wnp
www.trex-coe.eu

TREX
Targeting Real Chemical Accuracy at the Exascale

Enabling the community codes for stochastic quantum chemical simulations

Computers and the rapid mathematical calculations they are able to perform, which would take human beings years to accomplish, have enabled the fuel to power innovation. High-performance computing (HPC) and high-throughput computing (HTC) have enabled us to simulate large-scale complex processes and analyze tremendous amounts of data, benefiting applications ranging from climate research and drug discovery to material design. Emerging exascale computers will make the best even better, 50 times faster than today's most powerful supercomputers.

The TREX Center of Excellence (CoE) federates European scientists, High Performance Computing (HPC) stakeholders, and SMEs to develop and apply high-performance software solutions for quantum mechanical simulations at the exascale.

TREX Main Outcomes

- Co-design of computational codes with efficient scalable algorithms for HPC applications.
- Rational design of an ecosystem of highly scalable, optimized, and interoperable QMC codes.
- Robust management of complex scalable QMC workflows in high-throughput calculations.
- Foster wider access, usage, and uptake of knowledge in HPC via direct involvement of present and potential user communities via demonstrators.

TREX Codes

- TurboRVB**: Scalable RVB solver for ground state QMC simulation of both molecules and bulk electronic systems.
- CHAMP**: The Quantum Hybrid QMC/Orbital Package (CHAMP) is a novel hybrid method designed for accurate and/or cost-effective molecular dynamics.
- QMC-Chem**: QMC-Chem is a quantum chemistry package for molecules and clusters.
- TREXIO**: The TREXIO library provides the tool for defining user-friendly quantum, high-level multi-configuration ground state QMC energy calculations in any programming language.
- NECI**: The NECI package for full configuration interaction quantum Monte Carlo method is a portable software for molecules, clusters and periodic systems with chemical accuracy including large systems, density matrices, ground properties, etc.
- Quantum Package**: Quantum Package (QP) is a novel software framework for molecular dynamics simulation (QMCD) and ground state QMC simulation (QMC) with advanced features.
- GAMMCOR**: GAMMCOR is an accurate and efficient ground state QMC code.
- QMCL**: The QMCL library aims at providing a high-level framework representation of the architecture of Quantum Monte Carlo methods.

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TREX
Targeting Real Chemical Accuracy at the Exascale

Enabling the community codes for stochastic quantum chemical simulations

TREX Consortium

The TREX consortium is committed to building an efficient and state-of-the-art framework in HPC and exascale computing by developing an **integrated software platform**.

UNIVERSITY OF TWENTE, CNRS, SISSA, CHECA, UNIVERSITY OF VERSAILLES, MEGWARE, SAV, TRUST-IT SERVICES

Key figures
Start 01 OCT 2020 | End 30 SEP 2023

Join the **TREX Community** trex-coe.eu/contact-us

www.trex-coe.eu | @trex_eu | TREX Project | TREX Channel

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Figure 24 TREX pop-up banner and flyer

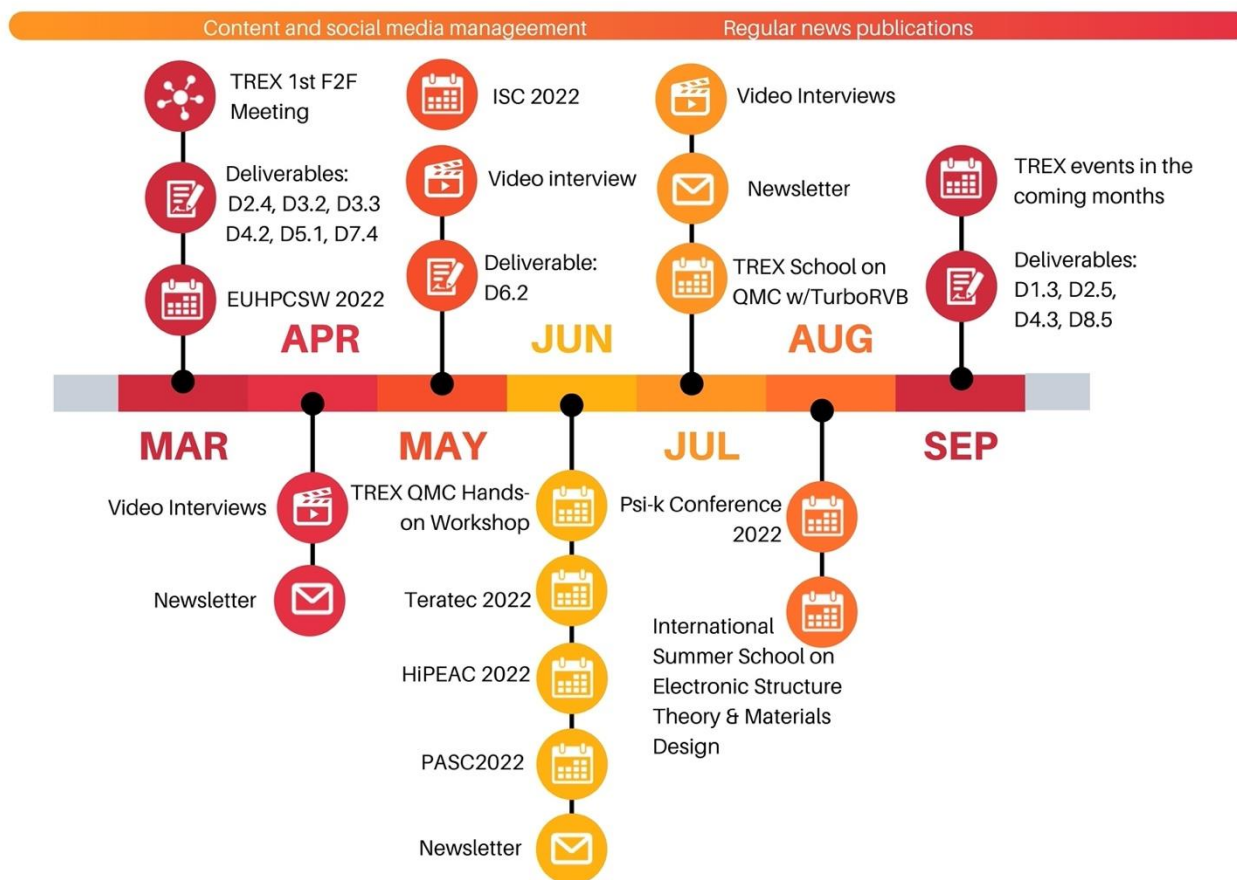
6. Conclusion

The TREX project is now moving to its second phase, where the development and consequent exploitation of the results and assets are expected. The communication, dissemination, and engagement plan will adapt to ensure continuous support to TREX training activities and the exploitation of the project assets.

The TREX team will also continue to join forces and establish synergies with relevant initiatives, EU-funded CoEs, and other HPC organisations to make the outcomes of the project as much available as possible and to reach out to the widest audience within the academia, industry, and policy arena.



ANNEX I - Timeline of activities from M19-M34



ANNEX II - List of TREX organised and participated events

Table 1: TREX events (M1-M18)

TREX Events			
Workshop and Schools, and Hackathons: 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 schools and more.			
Total number of organised events: 4 events			
Total number of participants: 164 participants			
Event	Date	Location	Audiences Reached

TREX e-School on Quantum Monte Carlo with TurboRVB	12-16 Jul 2021	Online event	Plenary attendees: 89 Hands-on participants: 24 Speakers and technical support: 3 speakers and 5 support from SISSA and CNRS/Paris
TREX session at the virtual PRACE booth at ISC 2021	24 Jun – 2 Jul 2021	Online event	Visibility to over 2000 international attendees and 84 exhibitors; 30 participants to the session
TREX Build-system hackathon	8-12 Nov 2021	Online event	Plenary attendees: 45 Hands-on participants: 22 Speakers and technical support: 9 speakers and 2 support from CNRS/Toulouse and UVSQ
TREX Hackathon II with TREX event at UVSQ	28 Feb – 4 Mar 2022	Versailles, France	TREX consortium



Table 2 – 3rd party event Events Participation to 3rd party events

HPC ecosystem events, including events organized by/with the HPC Center of Excellence Council (HPC3) and FocusCoE, or resulting from collaborations with other HPC CoEs, HPC advancement events, QMC and stochastic training events and domain-specific industry targeting research and academic audience including students, postdocs, researchers, industrial players, stakeholders working in public administrations.

	Event	Date, Location	TREX Representative
1	The importance of being H.P.C. Earnest (CECAM webinar series)	18 Jun 2020, Online event	UT, Claudia Filippi CNRS, Anthony Scemama
2	HPC3 Council	Jun 2020, Online event	UT, Claudia Filippi
3	CECAM2021 Workshop: Recent developments in quantum Monte Carlo	21-22 Oct 2020, Rome (IT)	CINECA, Fabio Affinito UT, Claudia Filippi CNRS, Michele Casula SISSA, Sandro Sorella
4	Tuning Workshop, Vi-HPS	7-11 Dec 2020, Online event	UVSQ, Cédric Valensi
5	Instructor training workshop for HPC CoEs	1 Nov 2020, Online event	UVSQ partner
6	Luchon Winter School - TREX Tutorials in Quantum Monte Carlo (QMC)	25 Jan - 8 Feb 2021, Online event	UT, Claudia Filippi CNRS, Anthony Scemama
7	3rd EMMC International Workshop	2-4 Mar 2021, Online event	CINECA, Fabio Affinito CNRS/Paris, Michele Casula
8	CoEs Co-Design Workshop	12 Mar 2021, Online event	CNRS, Anthony Scemama CINECA, Fabio Affinito
9	Helmholtz GPU Hackathon 2021 - Digital Event	15-24 Mar 2021, Online event	CNRS, Anthony Scemama SISSA, Sandro Sorella KTH, Dirk Pleiter
10	“Library development within TREX” at Gruneis’ Group (NOMAD), Vienna University of Technology	22 Apr 2021, Online event	CNRS, Anthony Scemama
11	CodeRefinery workshop	10-12 May 2021, Online event 18-20 May 2021, Online event	CNRS, Evgeny Posenitskiy TUL, Kasia Pernal KTH, Johan Hellsvik
12	10th ABINIT International Developer Workshop	31 May - 4 Jun 2021, Online event	UT, Claudia Filippi

13	ISC 2021	24 Jun – 2 Jul 2021, Online event	CNRS/Toulouse, Anthony Scemama UVSQ, Cedric Valensi, Pablo de Oliveira Castro, William Jalby
14	NCC-CoE meeting on First-Principle Simulations in Chemistry and Materials Science	1 Jul 2021, Online event	UT, Claudia Filippi CNRS/Toulouse, Anthony Scemama
15	Workshop on Ontologies for Materials-Databases Interoperability (OMDI2021)	5-7 Oct 2021, Online event	CNRS/Toulouse partner
16	NCC-CoE meeting on Code Optimization	1 Nov 2021, Online event	UVSQ, William Jalby
17	FocusCoE Centres of Excellence Webinar Webinar on the interaction with industries and SMEs	1 Dec 2021, Online event	Megware and CNRS/Paris partners
18	Stochastic Methods in Electronic Structure Theory	6-9 Dec 2021, Online event	UT, Claudia Filippi, Stuart Shepard, and Ramon Panades CNRS, Michele Casula SISSA, Sandro Sorella & Saverio Moroni
19	Luchon Winter School - TREX Tutorials in Quantum Monte Carlo (QMC)	24 Jan - 4 Feb 2022, Online event	UT, Claudia Filippi CNRS, Anthony Scemama
20	Girls Day University Twente	7 April 2022, Enschede, The Netherlands	3rd-party event (co-sponsored by TREX)

ANNEX III - List of publications by TREX participants (M1-M18)

Publication	DOI	Type
Calculation of Rényi entropy in realistic quantum systems	ARXIV https://arxiv.org/abs/2112.14199	Article
Energy Derivatives in Real-Space Diffusion Monte Carlo	DOI https://doi.org/10.1021/acs.jctc.1c00496	Article
Ground-state properties of the narrowest zigzag graphene nanoribbon from quantum Monte Carlo and comparison with density functional theory	ARXIV https://arxiv.org/abs/2111.06300	Article
Ultra-fast interpretable machine-learning potentials	ARXIV https://arxiv.org/abs/2110.00624	Article
Spin-Pure Stochastic-CASSCF via GUGA-FCIQMC Applied to Iron–Sulfur Clusters	DOI https://doi.org/10.1021/acs.jctc.1c00589 ARXIV https://arxiv.org/abs/2106.07775	Article

Publication	DOI	Type
Range-separated multiconfigurational density functional theory methods	DOI https://doi.org/10.1002/wcms.1566	Article
Probing anharmonic phonons by quantum correlators: A path integral approach	DOI https://doi.org/10.1063/5.0050450 ARXIV https://arxiv.org/abs/2103.04094	Article
Tailoring CIPSI Expansions for QMC Calculations of Electronic Excitations: The Case Study of Thiophene	DOI https://doi.org/10.1021/acs.ictc.1c00212 ARXIV https://arxiv.org/abs/2103.01158	Article
Localization versus inhomogeneous superfluidity: Submonolayer 4He on fluorographene, hexagonal boron nitride, and graphene	DOI https://doi.org/10.1103/PhysRevB.103.174514	Article
Spin-adapted selected configuration interaction in a determinant basis	ARXIV https://arxiv.org/abs/1812.06902	Article
Energy-free machine learning predictions of ab initio structures	ARXIV https://arxiv.org/abs/2102.02806	Article
Elucidating atmospheric brown carbon -- Supplanting chemical intuition with exhaustive enumeration and machine learning	DOI https://doi.org/10.1021/acs.est.1c00885 ARXIV https://arxiv.org/abs/2101.07301	Article
Machine Learning of Free Energies in Chemical Compound Space Using Ensemble Representations: Reaching Experimental Uncertainty for Solvation	DOI https://doi.org/10.1063/5.0041548 ARXIV https://arxiv.org/abs/2012.09722	Article
Ab initio machine learning in chemical compound space	DOI https://doi.org/10.1021/acs.chemrev.0c01303 ARXIV https://arxiv.org/abs/2012.07502	Article
TREX Targeting REal Accuracy at eXascale at CECAM Workshop	DOI 10.5281/zenodo.5720842	Presentation
TREX: an innovative view of HPC usage applied to Quantum Monte Carlo simulations	DOI 10.5281/zenodo.5061984	Presentation
Library development within TREX	DOI 10.5281/zenodo.4896769	Presentation
Guidelines for improving the performance of computer programs	DOI 10.5281/zenodo.4696165	Presentation
Software development strategy in the TREX Center of Excellence	DOI 10.5281/zenodo.4321302	Presentation
A new generation of HPC developers using quantum Monte Carlo (QMC) methods is growing	DOI 10.5281/zenodo.6364722	Report

