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D8.1 – Project Handbook

Version 1.0

GA no 952165

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Disclaimer



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Preface

The general principles for the project execution are defined in the EU Grant Agreement (GA), the Description of the Action (DoA), and the Consortium Agreement (CA). The Project Handbook does not replace any of these established agreements, nor does it replace any of the EU guidelines for project implementation and documentation.

In case of inconsistencies between these documents, the following order of precedence should be applied:

1. EU Grant Agreement including Description of the action, also referred to as the Grant Agreement (EU GA) Annex 1 [1];
 - a. Although the core contract is signed between the EU and the Coordinator of the project, all partners have become individual contract partners with the commission by signing the Accession Forms.
2. Consortium Agreement (CA) [3];
 - a. Whereas the Grant Agreement is signed between the EU and the partners, the Consortium Agreement is signed between the partners themselves. It arranges in more detail the provisions of the Grant Agreement, such as but not limited to financial issues, payments, management, decision making, conflict resolution, intellectual property rights and liability
3. Project Handbook (present document).



Document Revision History

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1.0	30-03-2021	J. Beerens (UT) and C. Filippi (UT)	First Official Release



Abbreviations

Abbreviation	Translation
UT	UNIVERSITEIT TWENTE
CNRS	CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE CNRS
SISSA	SCUOLA INTERNAZIONALE SUPERIORE DI STUDI AVANZATI DI TRIESTE
CINECA	CINECA CONSORZIO INTERUNIVERSITARIO
FZJ	FORSCHUNGSZENTRUM JULICH GMBH
MPG	MAX-PLANCK-GESELLSCHAFT ZUR FORDERUNG DER WISSENSCHAFTEN EV
UVSQ	UNIVERSITE DE VERSAILLES SAINT-QUENTIN-EN-YVELINES.
Megware	MEGWARE COMPUTER VERTRIEB UND SERVICE GMBH
STUBA	SLOVENSKA TECHNICKA UNIVERZITA V BRATISLAVE
UNIVIE	UNIVERSITAT WIEN
TUL	POLITECHNIKA LODZKA
TRUST-IT	TRUST-IT SRL
GDPR	General Data Protection Regulation
IPR	Intellectual property rights
NDA	non-disclosure agreement
PO	Project Officer
PM	Project Manager
WP	Work Package
WPL	Work Packager Leader
GA	Grant Agreement - 952165
CA	Consortium Agreement

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1 Introduction

In a few years, in Europe the first generation of exascale machines will exist. To harness this huge computational power, new software strategies need to be devised and this requires a significant, joint effort of domain scientists and computational experts. The TREX Centre 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. In quantum chemistry and materials science, it is extremely difficult for most methods to achieve exascale scaling and optimally exploit the precious resources which will become available. The quantum Monte Carlo approaches at the heart of TREX are among the few methods in the field of quantum simulations that can fully exploit the massive parallelism of future exascale supercomputers. The coupling of these advanced methods with exascale computing will enable simulations at the nanoscale of unprecedented accuracy, targeting a fully consistent description of the quantum mechanical electron problem for very large systems.

This Project Handbook describes how the management procedures and processes are defined and implemented within the TREX project. This includes the CoE governance structure and associated infrastructure, as well as the project operational guidelines. Management activities will be monitored within Work Package 8. Some sections are reused from the original proposal. The Handbook is a living document in that it will be updated as required throughout the project should possible improvements be identified, or an unforeseen risk occur.

This report is divided into multiple chapters. In Chapter 2, an overview of the project and of the key reporting periods to the European Commission are provided, as well as a summary of the milestones and deliverables. Chapter 3 describes the CoE Governance structure, the details of the associated infrastructure, and the different roles and associated responsibilities of the partners. The operational Guidelines are summarised in Chapter 4: these cover the way of reporting, the risk management procedure, the decision-making, and the conflict of resolution procedure, as well as the dissemination procedure. The report is concluded in Chapter 5.



2 Project Overview

In this Chapter, an overview of the entire project is presented. Section 2.1 gives the public summary and list the project beneficiaries. The reporting periods to the European Commission are detailed in Section 2.2. The project beneficiaries are listed in Section 2.3 and the key milestones and deliverables in Section 2.4. A breakdown of the project into Work Packages (WPs) is described in Section 2.5.

2.1 Project Summary

As described on the project website, the project can be summarised as follows [2]:

“The TREX Centre of Excellence (CoE) aims at developing, promoting, and maintaining open-source high-performance software solutions in the field of quantum chemistry, which are ready to take advantage of upcoming exascale architectures. TREX’s ambition is to predict experiments in silico at the nanoscale by means of advanced and systematically improvable stochastic methods targeting the faithful simulation of a fully consistent quantum mechanical electron problem.

To this aim, TREX will exploit and foster the use of supercomputers with energy-efficient accelerators (e.g., GPU) by means of state-of-the-art quantum Monte Carlo (QMC) codes, developed in Europe, and internationally recognized as key algorithmic assets.

TREX will facilitate access to the corresponding software suites with high quality documentation and user-friendliness. This will reduce the barrier between advanced numerical simulations and scientific and industrial applications, thus accelerating innovation as well as establishing European leadership in computational science.”

2.2 Reporting periods to European Commission

The project has a duration of 36 months and runs from October 1st, 2020 till September 30th, 2023. During this period, there will be 2 (two) formal reporting periods, occurring as shown in Table 1. Each period covers 18 months of the project. More details regarding the content of the reports can be found in Section 4.1.

Reporting to the European Commission and the Project officer will be carried out via the European participation portal accessible through the following link: <https://ec.europa.eu/info/funding-tenders/opportunities/portal/screen/home> The Portal is a password-protected environment in which specific rights are granted to the members of the consortium.

Table 1: Project Periodic Reporting Periods

What	Start of Reporting Period for all beneficiaries	Deadline for all beneficiaries	Deadline of Reporting Period towards EU
Periodic Report Period 1 (M01-M18)	01-04-2022	01-05-2022	31-05-2022
Periodic Report Period 2 (M19-M36)	01-10-2023	01-11-2023	30-11-2023

2.3 Project beneficiaries

Table 2 lists the beneficiaries with their country and website.

Table 2: Project Beneficiaries

No.	Abbr.	Beneficiaries name	Country	Website
1	UT	Universiteit Twente	NL	https://www.utwente.nl/en/
2	CNRS	Centre National de la Recherche Scientifique	FR	http://www.cnrs.fr/
3	SISSA	Scuola Internazionale Superiore di Studi Avanzati	IT	https://www.sissa.it/
4	CINECA	CINECA Consorzio Interuniversitario	IT	https://www.cineca.it/en/
5	FZJ	Forschungszentrum Jülich GMBH	DE	https://www.fz-juelich.de
6	MPG	Max-Planck-Gesellschaft zur Forderung der Wissenschaften EV	DE	https://www.mpg.de
7	UVSQ	Université de Versailles-Saint-Quentin-en-Yvelines	FR	https://www.uvsq.fr
8	Megware	Megware Computer Vertrieb und Service GmbH	DE	https://www.megware.com
9	STUBA	Slovak University of Technology in Bratislava	SK	https://www.stuba.sk/english.html
10	UNIVIE	Universität Wien	AT	https://www.univie.ac.at/en/
11	TUL	Politechnika Łódzka	PL	https://www.p.lodz.pl
12	TRUST-IT	TRUST-IT SRL	IT	https://www.trust-it-services.com
13	KTH	Kungliga Tekniska Hoegskolan	SE	https://www.kth.se/en

2.4 Milestones and Deliverables

Table 3 shows the Project Milestones as defined in the grant agreement. The Project Deliverables are visible for the members only [6].

Table 3: Project Milestones

Milestone	Month	Time	Means of verification
MS1	M06	Wednesday 31-03-2021	Plans and procedures ready
MS2	M12	Thursday 30-09-2021	First release of the libraries
MS3	M18	Thursday 31-03-2022	Interoperable software
MS4	M24	Friday 30-09-2022	Second release of the libraries
MS5	M36	Saturday 30-09-2023	TREX products fully developed

2.5 Project Breakdown

The project is divided into eight (8) Work Packages (WP), each covering a specific objective. Figure 1 provides a schematic overview of how the work packages are linked together. Each Work Package has a lead beneficiary and is subdivided into multiple tasks with corresponding task leaders. This information is only available for the participants of the TREX project [5]. Details on the various roles and responsibilities can be found in Section 3.2 “Milestones and Deliverables”.

The responsibilities and the tasks within a WP are assigned to different participants based on their specific competences. Importantly, the implementation of the WPs and tasks involves all beneficiaries in the Centre of Excellence. Furthermore, all partners are involved in the management activities as well as dissemination and exploitation activities.

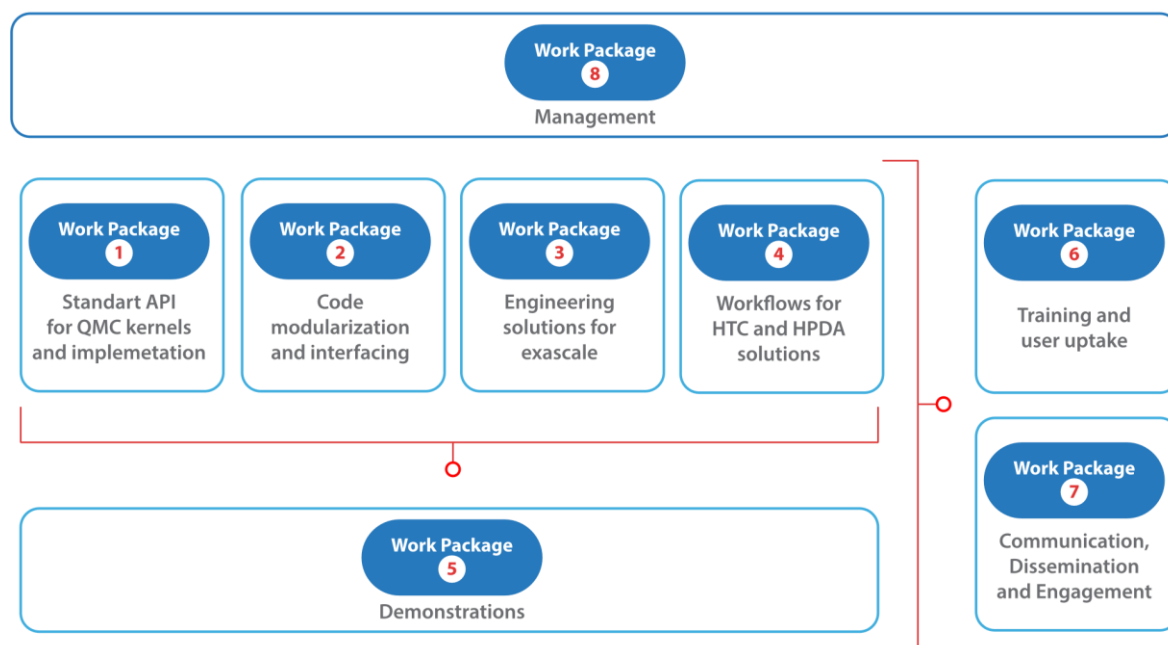


Figure 1: Overview of the Project Work Packages and the link between the Work Packages

WP1 lays down the core structure of our bid for exascale computing and takes the necessary steps to facilitate the creation of a high-performance kernel library for QMC (QMCKl) in WP3. WP1 establishes common design principles to develop an easy-to-read and easy-to-modify library which will enable a wide community of QMC experts, code owners, and newcomers to the field to quickly develop and test novel, cutting-edge mathematical formulations, and algorithms. WP1 will also enforce the implementation of quality control measures for exascale readiness, namely, a well-documented test suite to check all functions in QMCKl and a continuous integration system monitoring the numerical accuracy and the execution time.

WP2 aims to present users and developers with a platform of flagship codes, which seamlessly integrates their unique capabilities within an interoperable framework. This WP deals with the design of a common data format and its implementation in an I/O library, the modularization of the codes to incrementally take advantage of the I/O library and the QMCKl libraries. WP2 will also build a well-documented set of reference test cases for the main functionalities of the codes.

WP3 is concerned with the high-performance implementation of QMCKl, optimized for upcoming supercomputers, in co-design with the HPC partners. This WP will take care of the benchmarking and

profiling activities of TREX software with respect to different hardware features. WP3 will also explore and implement methods based on lower and mixed precision arithmetic's.

WP4 focuses on the development of robust workflows to enable users to easily perform standardized QMC calculations, operate TREX codes in a pipeline, and work in high-throughput computing (HTC) fashion when using exascale resources for machine learning purposes. In this context, WP4 also develops tools to help exascale HPC centres to go beyond their traditional usage models, with advanced provisioning services facilitating the new workflows for the QMC community. The WP also includes the algorithmic work needed to address new problems which will arise when going from petascale to exascale, e.g., higher probability of failure or problems related to large-scale communications.

WP5 will test and demonstrate the effectiveness of TREX software, its suitability for the exploitation of pre-exascale architectures also in HTC mode, and its readiness for the upcoming exascale computing generation. To this aim, TREX target applications, which are scientific and HPC challenges and address major societal priorities. Each "demonstration" is organized in layers of progressive complexity, reflecting the parallel development in TREX code portability towards newly deployed HPC infrastructures. Importantly, they will serve as invaluable feedback to WP1-4 by identifying possible problems and bottlenecks during the project.

WP6 coordinates the structured training and educational activities of TREX. These cover technical support to end-users of TREX software, hands-on training for code users in academia and industry, and hands-on workshops to forge a new generation of code developers. Special attention is given to the engagement of communities in countries currently developing their HPC ecosystem. WP6 will also target the education of young pupils and university students by developing a visual and modular tool for stochastic quantum simulations as well as coupling a yearly satellite event to a wide European school for master students.

WP7 will deliver and maintain TREX communication, Marketing and Dissemination Strategy. This includes the development of TREX graphic design and branding, TREX web platform as a single public portal to all TREX products, as well coordinated, continuous set of actions to ensure coverage of all stakeholders and adequate visibility worldwide. WP7 will engage in targeted communication and dissemination activities as well as in monitoring the uptake of TREX main assets. WP7 aims at increasing the pool of users and engaged stakeholders and promoting synergies within the EU HPC ecosystem for the exploitation and sustainability of the software beyond TREX.

WP8 will guarantee the coordination of TREX activities, the quality of the project outcomes and the definition of a long-term sustainability plan for the CoE. Operational activities include day-to-day management and monitoring of the project (administrative, technical, and financial), monitoring of adherence to the work plan, control of resources and timing, interaction with the EC and relevant external actors, and quality monitoring. WP8 will support the establishment and development of TREX in terms of governance structure and sustainability plan.



3 CoE Governance Structure and associated infrastructure

The general structure of the Centre of Excellence Governance is illustrated in Figure 2, which shows the TREX stakeholders and their interactions. The associated infrastructure is further detailed in Section 3.1, while the roles and responsibilities of the partners are described in Section 3.2. How the different bodies interact is discussed in Section 3.3.

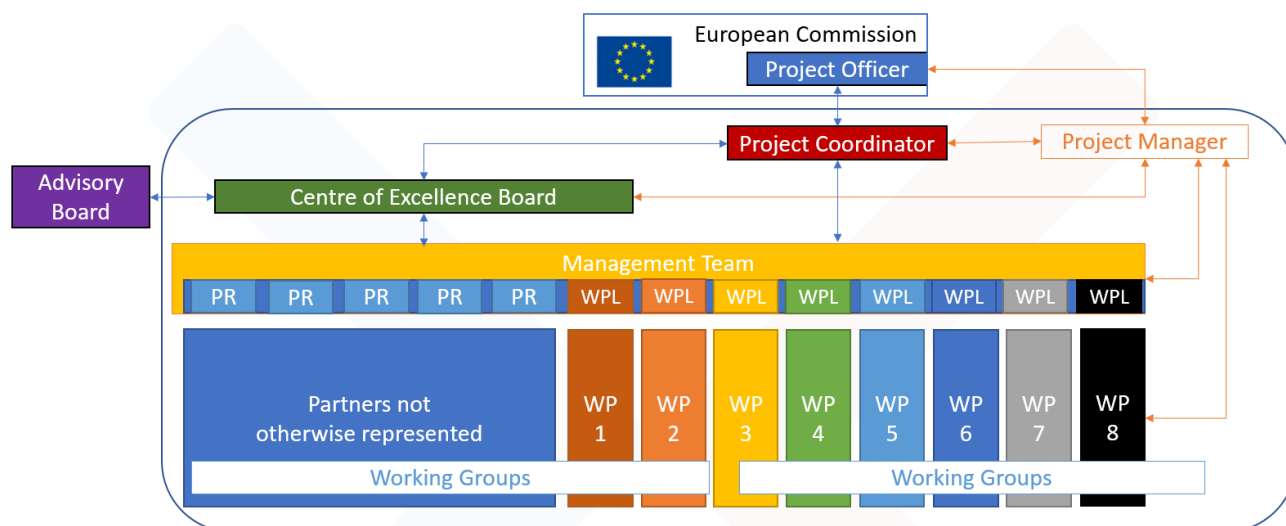


Figure 2: Organisational Chart with communication links indicated by arrows.

3.1 Associated infrastructure

The flagship codes of TREX are listed in Table 1 and comprise quantum Monte Carlo (QMC) as well as high-accuracy deterministic codes. These codes will be modularized and integrated with the QMCKl library developed within TREX; and will constitute an inter-operable platform of high-performance elements bringing accurate quantum mechanical simulations to the exascale.

Table 4: TREX flagship codes

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

The consortium will regularly apply for computational resources via PRACE and the various national facilities.

3.2 Roles and responsibilities

3.2.1 European Commission with Project Officer

The European Commission (EC) is represented by a Project Officer (PO) to ensure the correct implementation of the Grant Agreement. The Project Officer (PO) is responsible for the review of all the deliverables, the periodic reporting, and all communication with the European Commission. The Project Officer (PO) is assisted by a Financial Officer of the European Commission.

Formal communication with the Project Officer is done via the EU Portal.

3.2.2 Project Coordinator

Claudia Filippi from the University of Twente is appointed as Project Coordinator (PC) and is responsible for ensuring the appropriate and efficient management, coordination, and progress of the activities. The Project Coordinator is assisted by the Project Manager (PM).

The responsibilities of the Project Coordinator (PC) include:

- Acting as point of contact between the Centre of Excellence, the European Commission, and other relevant external bodies as for instance FocusCoE and HPC3.
- Coordinating collective responsibilities within the Centre of Excellence and monitor contractual obligations.
- Ensuring timely reporting, e.g., deliverables and periodic reporting to the European Commission regarding technical and financial matters.
- Chairing the CoE Board and Management Team meetings.
- Chairing the Advisory Board meetings.
- Facilitating the scientific progress of the project.
- Encouraging frequent and effective communication among the members of the Centre of Excellence and motivate their active participation in all activities.
- Communicating with the Work Package Leaders to identify possible delays in the deliverables and monitoring the milestones. In case of deviations from the original plan, acting in coordination with the Management Team.

3.2.3 Project Manager

Jan Beerens from the University of Twente is appointed as Project Manager (PM) and will assist the Project Coordinator (PC) in the day-to-day management of the project.

The Project Manager will have a special role in consolidating the project planning, progress reports, deliverable and milestone reports, cost statements, and budget. He will facilitate all managerial aspects of the project so that the Project Coordinator can also focus on the scientific tasks.

The responsibilities of the Project Manager (PM) include:

- Assisting in the organisation of the meetings such as Kick-Off, Management Team, CoE Board, and Advisory Board Meetings.
- Submitting the deliverables and communicating with the Project Office via the European Portal.
- Promoting effective communication between the partners.
- Facilitating the managerial aspects of the project.
- Tracking the Risk Log and the Decision Log.



3.2.4 Centre of Excellence Board

Each partner has a representative in the CoE Board. The main responsibilities of the Board are to guard the strategic direction and vision of the CoE. Any strategic formal decision regarding the present and future of the CoE will be taken by the CoE Board [1][3]. The Board members will be briefed and advised by the Management Team. The Board only meets if a decision is required regarding the evolution of the consortium and possible changes to the content, finances, and intellectual property rights confirm the consortium agreement. The Board will also meet when a specific case of conflict cannot be resolved by the Management Team (see Section 4.4).

3.2.5 Management Team

The Management Team consists of the Project Coordinator, assisted by the Project Manager, the Work Package Leaders, and a representative of any beneficiary that does not lead a Work Package (see Figure 2). Table 5 gives an overview of the members in the Management Team, their role, and their organisation. With such a composition, cooperation between all partners is assured and all beneficiaries are represented (being for instance able to vote) during the relevant meetings. The Management Team is responsible for ensuring the compliance of the activities with the scope of the project, for the timely completion of the project deliverables including (periodic) reporting as well as for financial and legal issues. The Management Team advises the CoE Board and is responsible for the implementation of the decisions of the CoE Board. The Management Team is the body to which the Work Packages and Working Groups report. A main responsibility of the Management Team is to ensure compliance with the Grant and Consortium Agreements.

Table 5: Members of the Management Team

Attendee Name	Initials	MT Role	Organisation	Voting Rights ¹
Claudia Filippi	CF	Project Coordinator	UT	Yes
Jan Beerens	JB	Project Manager	UT	No
Anthony Scemama	AS	WP1	CNRS	Yes
Michele Casula	MC	WP5	CNRS	No
Sandro Sorella	SS	WP2	SISSA	Yes
Fabio Affinito	FA	-	CINECA	Yes
Dirk Pleiter	DP	WP3	FZJ	Yes
Ali Alavi	Aal	-	MPG	Yes
William Jalby	WJ	-	UVSQ	Yes
Axel Auweter	Aau	-	Megware	Yes
Matus Dubecky	MD	WP6	STUBA	Yes
Anatole von Lilienfeld	AvL	WP4	UNIVIE	Yes
Kasia Pernal	KP	-	TUL	Yes
Sara Pittonet Gaiarin	SP	WP7	Trust-IT	Yes
				12/14

The Management Team will meet monthly. The Project Coordinator and Project manager prepare the agenda for each meeting. The general outline of the agenda is set in following way: overall TREX status update by PC and PM; status updates of Work Packages by the WPL; discussion based on the

¹ Each beneficiary has one (1) vote. The PM has no voting rights.

current status to evaluate the past actions and define the following steps. Each member of the Management Team can add a topic to the agenda by informing the PC and PM.

During the project, additional and special roles can and will be assigned within the Management Team if required. This will be regularly monitored and updated. Currently defined roles are:

- Monitoring the progress towards Exascale:
 - Anthony Scemama will be the primary responsible person with special focus on the chemistry aspect and,
 - William Jalby will act as secondary responsible person with special focus on the High-Performance Computing aspects.
- Other roles can be defined.

3.2.6 Work package leader

A Work Package Leader oversees a specified Work Package. The Work Package Leader is responsible for all scientific and managerial progress. Work Package leaders are among TREX principal investigators (PI). The Work Package Leader will be responsible to take appropriate actions to ensure work progress, and to implement any decisions by the Management Team. Work Package leaders will not only monitor the activities within their Work Package but, whenever necessary, be also responsible for the coordination of actions towards the common goals of the CoE. In this respect, within their dedicated areas, Work Package leaders will monitor the development of activities of general importance to the CoE (e.g., activities involving interaction with external stakeholders) and will watch out for opportunities that may benefit the CoE development and sustainability.

The Work Package Leaders will setup regular meetings with all participants to discuss progress and ensure traceability of the decisions. They will set up an agenda for the scientific meetings, take minutes of the meetings, and follow-up all the actions within the Work Package.

3.2.7 Task Leader

The task leader is selected based on his/her specific competences and is responsible for a specific task defined within the Work Package. Together with the Work Package Leader, the task leader is responsible for the scientific work executed within the task. The task leader is also responsible for timely and proper reporting of the actions. The task leader works in close collaboration with the Work Package Leader and the individual collaborators involved in the task.

3.2.8 Work Package Members

The members of each Work Package will execute the scientific work. Each partner involved in the Work Package will designate one representative to each Work Package to act as contact person. All members can send a topic for discussion at a Work Package meeting to the WPL.



3.2.9 Advisory board

An Advisory Board to the CoE will be established. The Advisory Board will play an important role by supporting the CoE in its scientific directions as well as in legacy and sustainability strategy. The Advisory Board will closely interact with the CoE Board. The Advisory Board will include internationally renowned experts in quantum mechanical simulations and/or HPC, from academia and industry. See Table 6 for the current composition of the Advisory Board. The Centre of Excellence will regularly check if it is beneficial to include additional members in the Advisory Board.

The Coordinator shall take the minutes of the Advisory Board meetings and ensure that the suggestions of the Advisory Board are implemented. The Advisory Board members can be invited by the CoE Board to join a CoE Board meeting, but the Advisory Board does not have voting rights. The members of the Advisory Board will have a non-disclosure agreement (NDA) with the consortium.

Table 6: Members of the Advisory Board

Name	Organisation	Country	Function
Prof. Nicola Marzari	EPFL	Switzerland	Director of the NCCR MARVEL Swiss centre on computational Design and Discovery of Novel Materials.
Dr. Eric Petit	Intel Corporation	France	Parallel programming and numerical accuracy expert.
Prof. Peter Gill	Sydney University	Australia	Member of Board of Directors of QChem.
Dr. Paul Kent	Oak Ridge National Laboratory	USA	Principal investigator of QMCPACK.

3.3 Project Meetings and Collaboration Tools

3.3.1 Project Meetings

To ensure efficient communication and technical progress, internal meetings will be held on a regular basis as detailed in Table 7. These meetings are mainly aimed at monitoring general progress, namely, status of the actions, bottlenecks, risks, and issues. Planning, documents, and deliverables, etc. The appropriate representatives will take part in the meetings according to the Consortium Agreement. Where possible, project meetings will be combined with events like major scientific conferences or TREX events, thereby optimizing communication. Regular communication between individual participants is encouraged in all possible ways by means of face-to-face meetings, regular phone calls, or online meetings.

Table 7: Overview of Recurring Meetings

	Reoccurrence	Note
CoE Board Meeting	At least every 1 year	If necessary
Advisory Board Meeting	Every 6 months up to 1 year	
Management Team Meeting	Every 4 weeks	
Work Package Meetings	Every 2 weeks	
Consortium meetings	After every milestone	Preferable during one of the TREX events.
First Periodic Reporting Meeting	M18 - M20	
Second Periodic Reporting Meeting	M36 - M38	

3.3.2 Online Platforms

As the online platform for storing official and internal documentation, MS Teams has been selected and a TREX Team is setup in the environment hosted by the University of Twente. Figure 3 shows a screenshot of the MS Teams environment, which is only accessible to members of the Centre of Excellence. All relevant information is stored within the General Tab sections. This includes an overview with quick links to meetings and source codes, the agenda, the list of TREX participants, information regarding all the meetings, templates and logo, official documentation such as proposal, grant and consortium agreements, final deliverables. A dedicated TREX MT channel is setup to store all information regarding the Management Team meetings. For each Work Package, a separate channel has been created to post communication, store information, and collaborate on the deliverables. Each Work Package Leader is responsible for the content of the WP folders.

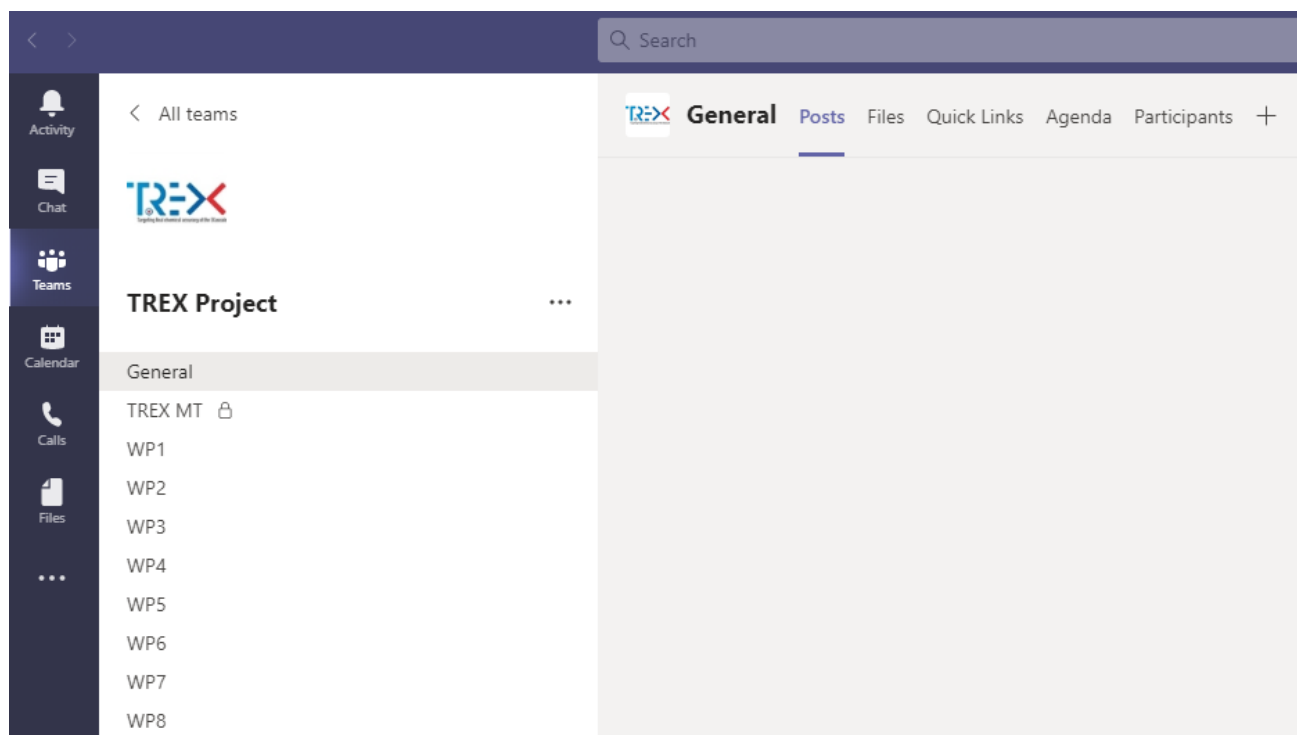


Figure 3: Screenshot of the TREX environment within Microsoft Teams

A dedicated environment for the different source codes has been setup on <https://github.com/TREX-CoE> which is only accessible to the members of the Centre of Excellence.

3.3.3 Internal Mailing lists

Multiple e-mail mailing lists have been setup to facilitate internal communication. Only members added to the mailing lists are enabled to send e-mails through the TREX mailing lists. In the online Teams environment, an excel file is available with all participants and their contact information. The file also shows which members are listed in the individual mailing lists.

Table 8: Overview of Internal mailing lists

e-mail address	Purpose
An e-mail address is available to TREX members only	All internal members of TREX
Multiple e-mail addresses are available to TREX members only	Communication to the individual work packages WP1 – WP8
Other e-mail addresses are available to TREX members only	e.g., Management Team, Editorial Team or other required for internal communication.

3.3.4 External communication

The reader is addressed to the publicly available² deliverable D7.1 – “TREX Branding and communication kit” for all details on templates, communication etc. The most important communication channels are shown below and the logo of TREX is given in Figure 4.

- <https://www.trex-coe.eu/>
- https://twitter.com/trex_eu with @trex_eu
- <https://www.linkedin.com/company/trex-eu/>



Figure 4: TREX logo

² After approval by the European Commission

4 Project Operational Guidelines

4.1 Reporting

4.1.1 Periodic Reporting

As mentioned in Section 2.2, the periodic reporting consists of a Technical Report and a Financial report. The individual partners will share the relevant information with the Project Manager so that he can timely deliver these reports to the European Commission. The overall structure of these reports is described below, and further details can be found on the website of the European Commission[4].

Technical report

The technical report is divided into 2 parts:

Part A: structured tables from the grant management system:

- cover page,
- summary for publication,
- web-based tables covering issues related to the project implementation (e.g., work packages, deliverables, milestones, etc.),
- answers to the questionnaire about the economic and social impact, especially as measured against the Horizon 2020 key performance indicators and monitoring requirements.

Part B: free text, core part of the report that one must upload to the grant management tool under the Report Core tab, as a single PDF document with:

- explanations of the work carried out by all beneficiaries and linked third parties during the reporting period,
- an overview of the progress towards the project objectives, justifying the differences between work expected under Annex I and work performed, if any.

Financial report

It consists of structured forms from the grant management system, including:

- individual financial statements (Annex 4 to the GA) for each beneficiary (and third parties),
- explanation of the use of resources and the information on subcontracting and in-kind contributions provided by third parties, from each beneficiary for the reporting period concerned,
- periodic summary financial statement including the request for interim payment.

4.1.2 Obligation to keep records and other supporting documentation

Each beneficiary is responsible for the correct implementation of the grant agreement and, according to Section 18.1 [1]:

The beneficiaries must — for a period of five years after the payment of the balance — keep records and other supporting documentation in order to prove the proper implementation of the action and the costs they declare as eligible.

They must make them available upon request (see Article 17) or in the context of checks, reviews, audits, or investigations (see Article 22).

If there are on-going checks, reviews, audits, investigations, litigation, or other pursuits of claims under the Agreement (including the extension of findings; see Article 22), the beneficiaries must keep the records and other supporting documentation until the end of these procedures.

The beneficiaries must keep the original documents. Digital and digitalised documents are considered originals if they are authorised by the applicable national law. The Commission may accept nonoriginal documents if it considers that they offer a comparable level of assurance

Special care should be taken with respect to the hour registration for supporting the personnel costs. The partners must keep time records for the number of hours declared and ensure that a reference to the Work Package is made to easily verify that the work carried out matches the work assigned and the person-months reported to the action. Information included in timesheets must match records of annual and sick leave taken and work-related travel.

4.1.3 Financial - Central budget for coordination

The project has received a central budget related to associated cost for coordination. To this aim, in accordance with the beneficiaries, the UT will keep a central budget for the consortium to support:

1. organisational costs of all these activities,
2. bursaries to support the participation of young(er) scientists, from countries currently developing their strategies and capacities, for integrating the HPC ecosystem,
3. childcare costs for female participants and single parents attending TREX events with young children,
4. travel costs of the Advisory Board members,
5. costs of invited speakers/lecturers etc.

When beneficiaries use this budget, first they will consume their own budget within “D. Other direct costs”. If budget is exceeded, a transfer of budget will be performed from the central budget to the beneficiaries. The beneficiaries should report and show their actual spending towards the coordinator.

4.1.4 Quality Control for deliverables to European Commission

Selection of Reviewers

Each deliverable has at least 2 reviewers, namely, one reviewer from within the Work Package and one reviewer from another Work Package to ensure alignment within a Work Package and across Work Packages. The primary investigators (Work Package leaders or task leaders) are selected as reviewers.

Timeline for review process

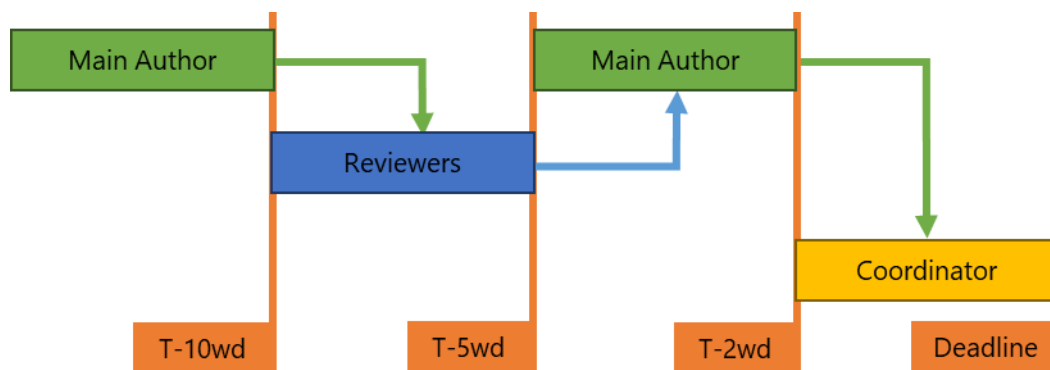


Figure 5: Timeline for review process

To illustrate the timeline of a review process, an example is given of a deadline on 30 November 2020:

- Fri 13-11-2020 > Deadline for submitting to reviewers the final draft.
- Fri 20-11-2020 > Deadline for submitting feedback to author.
- Wed 25-11-2020 > Deadline for submitting to Project Manager.
- Mon 30-11-2020 > Deadline for submitting to EU.



Definition for naming the document

Draft Naming: TREX-<Number of Deliverable> <Title> <Version> <Participant>

<Title>	D8.1
<Number of Deliverable>	Project Handbook
<Version>	V0.1
<Participant>	Lead Author; Contributing Author; Reviewer

Draft version e.g., TREX-D8.1-Project-Handbook-V0.1-JB

In the final, released, version, the <participant> is omitted.

Final Version e.g., TREX-D8.1-Project-Handbook-V1.0

Definition for versioning

The version number has the style VX.Y.Z. Where:

- V is short for version,
- X is defined and incremented by the Project Coordinator / Project Manager,
- Y is defined and incremented by the lead author or contributing author(s) of the document,
- Z is defined and incremented by the reviewers/

Examples:

- V0.0 is the template filled by the Project Manager for a given deliverable,
- V0.1 is the initial document by the main author,
- V0.# is a subsequent update of the document by the lead author or a contributing author,
- V0.1.# is version after review by one of the two reviewers,
- V#.0 is an official release to the European Commission by means of the Portal, performed by the Project Coordinator (with assistance of the Project Manager).

Note: Only a version with naming V#.0 will be submitted to the European Commission. The versioning and contribution history will be updated by the Project Manager to only include the final versions.

Review process

The reviewers should act as peer reviewers checking whether the content is scientifically correct, and the task is carried out according to the grant agreement. Furthermore, they should ascertain confidentiality issues. If the document is publicly available, they should make sure that the document is easy to read for the public. The reviewers should not rewrite the documentation but point out to the lead author suggestions for changes and possible improvements.

4.2 Risk Management Procedure

During the project lifetime, it is possible that a risk is identified which needs to be mitigated to avoid negative repercussions on the execution of the project.

The Project Manager is responsible for collecting the risks within a Risk Log. Each identified risk will be given a unique number. Its description and the person who identified the risk will be recorded in the Log.

During the risk assessment, the likelihood (L) of occurrence and impact (I) after occurrence will be determined and be quantified with a number, where 5 is very high and 1 is very low. The risk level is the combination of the likelihood (L) and impact (I). Depending on the value of the risk level, a risk response strategy is defined which can range from avoiding the risk by modifying the project plan, reducing the risk by taking pro-active risk reduction activities (i.e., taking preventive measures), or accepting the risk after which a contingency plan and/or crisis communication plan should be detailed (i.e., preventive measures). It is also possible to transfer or share the risk with other entities such as insurance or others. During the risk assessment, a risk owner will also be identified who is responsible for managing the implementation of the response strategy and monitoring the risk.

As to practical implementation, each person within the consortium should pro-actively identify a potential risk to the Work Package Leader and the Project Manager. The first risk response strategies are to avoid and/or reduce the risk. If after the first assessment, the Risk number is still larger than 8, the Management Team will be informed. During the subsequent Management Team meeting, a new risk assessment will take place to detail the risk reducing strategy.

4.3 Decision-making procedure

During the project, collaboration between partners might trigger adjustments or fine-tuning of some activities. Decisions and agreements need to be transparent and traceable for the entire Centre of Excellence during the entire duration of the project. Agreement may be reached first by informal contact, followed by official confirmation via electronic mail, letter, or agreed written minutes. Non-technical factors such as resource allocation and contractual terms will also need to be agreed and documented in writing.

The Project Manager is responsible for keeping a Decision-making Log.



4.4 Conflict resolution procedure

In every work situation, conflicts might occur. Most conflicts can be easily resolved among the persons involved. However, when solving a conflict is considered difficult, a conflict resolution procedure is setup.

Work Package Leaders will inform the Management Team of any potential conflict situation. Technical issues/conflicts will be tackled and solved at WP level, unless they involve a change of contract, a change of budget, and/or a change of resources/overall focus. If the decision being taken is unacceptable to partners found in the minority position, the resolution of the conflict will be escalated according to the procedure which is summarized in the following steps:

- First, the members of the WP concerned will inform the WP leader and Project Manager about the conflict occurred.
- As soon as the WP leader becomes aware of a conflict, the WP leader will convene a WP team meeting to discuss the issue. In case of agreement, the WP leader will inform the Management Team.
- If no decision is taken, the WP leader will inform the Management Team. The latter will contact the relevant persons and intervene to help resolve the conflict.
- Any unresolved issue will be escalated to the CoE Board.
- The next level of escalation as described in the Consortium Agreement is mediation in accordance with the WIPO Mediation Rules. The place of mediation shall be Brussels unless otherwise agreed upon. The language to be used in the mediation shall be English unless otherwise agreed upon [3].
- If, and to the extent that, any such dispute, controversy or claim has not been settled pursuant to the mediation within 60 calendar days of the commencement of the mediation, the courts of Brussels shall have exclusive jurisdiction [3].

4.5 Intellectual property rights (IPR)

The Intellectual Property Rights (IPR) are defined and agreed in the signed Consortium Agreement (CA) version 2 – 2020-10-21).

Background

Any details concerning the access rights to Background for the duration of the project are defined in the CA. Access to background can be requested in writing to a partner.

Patents

If patents are applied for, the partner will inform the consortium at the MT meeting. If applicable, the partner will disclose:

- Type
- Whether or not the application is confidential
- Application title
- A possible embargo end date.
- Application code
- IPR common data

Data Management Plan

The Data Management Plan will be detailed in a separate deliverable D8.2 “TREX Data Management Plan” which will be confidential to the members of the consortium and the Commission.



4.6 Dissemination

Section 4.6.1 summarizes how the European Commission will be acknowledged. The dissemination procedure is detailed in Section 4.6.2. The General Data Protection Regulation (GDPR) is described in Section 4.6.3. The position of the TREX Data Controller officer is elaborated in Section 4.6.4.

4.6.1 Acknowledgement

All external communications should comply to the EU acknowledgment regulations regarding the disclaimer and use of logo. The reader is referred to the Grant Agreement in articles 27.3, 28.2, 29.4, and 38.1.2. Within the TREX project, the following sentence and EU logo should be added:

1) Papers:

a. *“This work is supported by the European Centre of Excellence in Exascale Computing TREX - Targeting Real Chemical Accuracy at the Exascale. This project has received funding from the European Union’s Horizon 2020 - Research and Innovation program - under grant agreement no. 952165.”*

OR

b. *“This work is partially supported by the European Centre of Excellence in Exascale Computing TREX - Targeting Real Chemical Accuracy at the Exascale. This project has received funding from the European Union’s Horizon 2020 - Research and Innovation program - under grant agreement no. 952165.”*

OR

c. Similar formulation.

Optionally, one can add:

“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.”.

2) Talks and Posters

a.  [TREX LOGO]

AND

b.  [the EU emblem]

AND

c. *“The European Centre of Excellence in Exascale Computing TREX - Targeting Real Chemical Accuracy at the Exascale – has received funding from the European Union’s 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.”*

Optionally, one can add the logos of the beneficiaries within TREX.

These logos can be found at the protected MS Teams environment.

4.6.2 Dissemination procedure

During the Project and for a period of one (1) year after the end of the Project, the dissemination of own Results by one or several Parties including but not restricted to publications and presentations, shall be governed by the procedure of Article 29.1 of the Grant Agreement subject to the following provisions.

Prior notice of any planned publication shall be given to the other parties at least fourteen (14) calendar days before the publication. Any objection to the planned publication shall be made in accordance with the Grant Agreement in writing to the Coordinator and to the party or parties proposing the dissemination within fourteen (14) calendar days after receipt of the notice. If no objection is made within the time limit stated above, the publication is permitted.

Communication and dissemination activities to be carried out within the framework of WP7 of the TREX Consortium as part of the Communication, Marketing and Dissemination Plan (e.g., on the spot news articles, news-pieces as well as social media posts) shall be exempted from this provision in order not to impede the Project's dissemination strategy. This does not exempt the disseminating Parties from their obligations of Confidentiality under Section 10 of the Consortium Agreement.

During the kick-off meeting, it was agreed that if a partner stays silent, it is assumed they have no objections to publication. The partner will send the final version of the action to all partners for a final approval. Again, if partners stay silent, it is assumed they approve of the publication.

4.6.3 GDPR

TREX partners will comply with the respective national laws and regulations concerning protection of personal data, which are in line with the Regulation (EU) 2016/679 of the European Parliament and of the Council of 27 April 2016 on the protection of natural persons with regard to the processing of personal data and on the free movement of such data (GDPR), and repealing Directive 95/46/EC (General Data Protection Regulation) and the Convention 108 for the Protection of Individuals with Regard to Automatic Processing of Personal Data (as well as Regulation (EU)).

For the research activities, no collection of personal data is required. The personal data of participants in TREX initiatives will be collected and processed for the sole purpose of implementing, managing, and monitoring the activities organized during the project. These activities may imply actions like registration in courses/webinars, attendance lists, consent forms, potential assignments, and assessment forms. Personal data will be collected at the minimum possible level to allow the implementation of the relevant TREX activities (i.e., in accordance with the "data minimisation" principle)[1].

4.6.4 TREX Data Controller

Each partner is responsible to comply with the provisions of the GDPR and to respect the European ethical rules and standards, including those reflected in the Charter of Fundamental Rights of the European Union. No project specific Data Protection Officer (DPO) needs to be appointed and no Data Processing Agreement (DPA) needs to be signed.

In compliance of the before mentioned GDPR, public institutions that are part of TREX have appointed a Data Protection Officer (DPO):

Short name	Local DPO contact



UT	https://www.utwente.nl/en/news/2019/4/328975/new-data-protection-officer
CNRS	http://www.cnrs.fr/en/rgpd
SISSA	https://www.sissa.it/privacy
CINECA	https://bestr.it/privacy?ln=en
FZJ	https://www.fz-juelich.de/portal/EN/dataprotection/_node.html#doc927660bodyText14
MPG	https://www.mpg.de/privacy-policy
UVSQ	http://www.uvsq.fr/mentions-legales-uvsq-235076.kjsp?RH=1188915773029
STUBA	https://www.stuba.sk/english/university/contacts/conditions-of-privacy-protection.html?page_id=12412
UNIVIE	https://www.wu.ac.at/en/datenschutz
TUL	http://bg.p.lodz.pl/en/privacy-policy
KTH	https://www.kth.se/profile/rroy
Trust-IT	Michele Nannipieri

5 Conclusions

This Handbook presented the Governance Structure and the operational guidelines for the TREX Centre of Excellence in Exascale Computing.

The governance structure was overviewed, and the roles and responsibilities of the various stakeholders defined. The project meetings and the tools setup to ensure effective communication and collaboration were described in detail.

Various operational guidelines were clarified (e.g., the reporting procedure to the European Commission) to ensure that all members of the consortium are aware of the regulations and requirements. These include the obligation to keep records and other supporting document, the rules for distributing the central TREX budget, and the quality control procedure.

Some managerial procedures as risk management, decision-making, conflict resolution procedures and the intellectual property rights were also explained. Finally, the dissemination procedures were given.

This document will be updated during the project as required.



References

- [1] Project Grant Agreement - 952165
- [2] Project Website, <https://trex-coe.eu/>
- [3] Project Consortium Agreement version 2 – 2020-10-21.
- [4] https://ec.europa.eu/research/participants/docs/h2020-funding-guide/grants/grant-management/reports/periodic-reports_en.htm
- [5] TREX Project Participants List.xlsx on the MS Teams environment, confidential to members of the consortium only.
- [6] TREX_Deliverables_Review_List.xlsx on the MS Teams environment, confidential to members of the consortium only.

