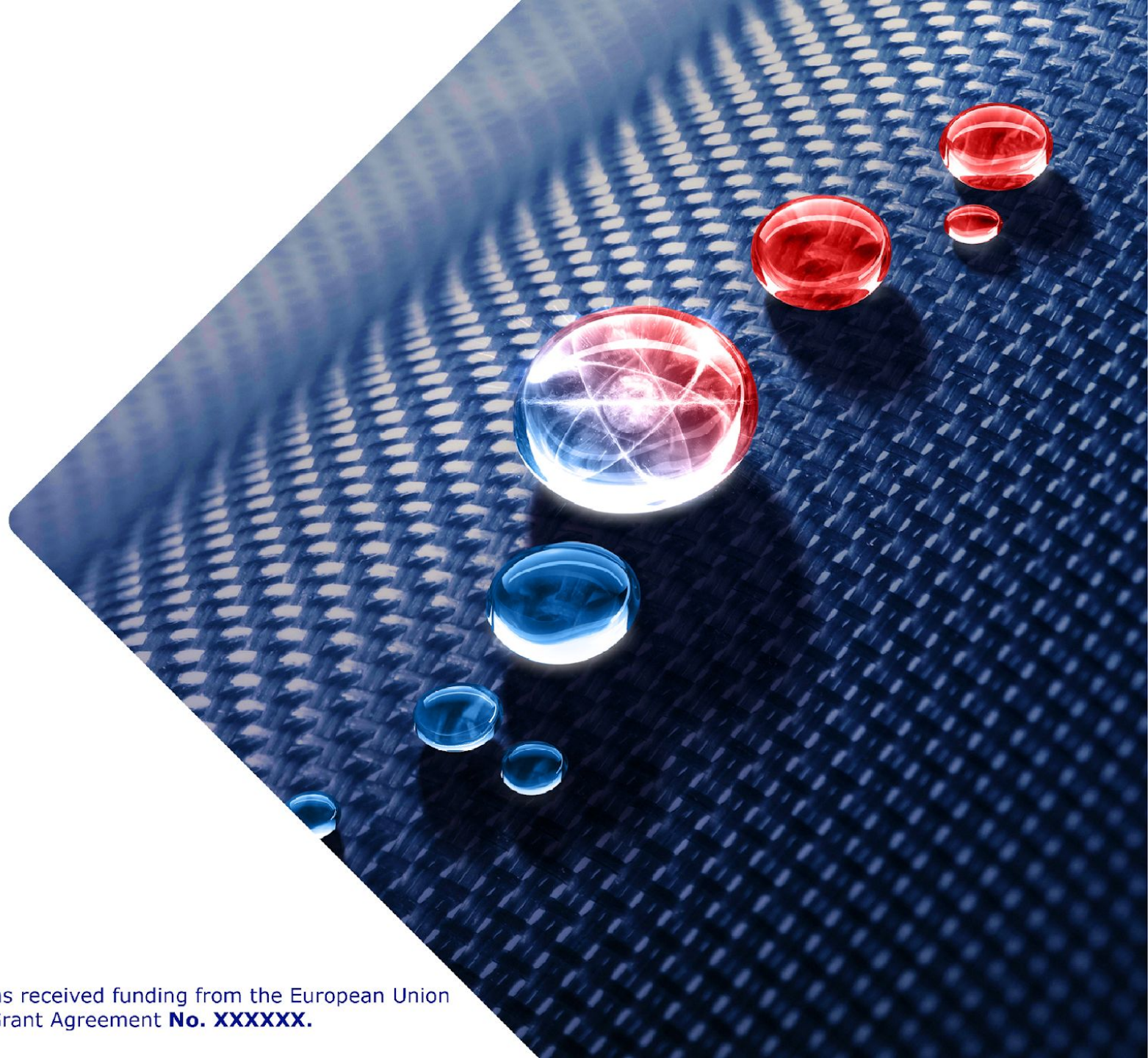
Targeting Real chemical accuracy at the EXascale

All Hands Status Overview

Outreach, exploitation & training WP6 & WP7

Sara Pittonet, Julie Arteza, Jacopo Mariani, Trust-IT
Fabio Affinito (CINECA)
Ivan Stich, IPSAS



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

Targeting Real chemical accuracy at the EXascale

TREX Community overview

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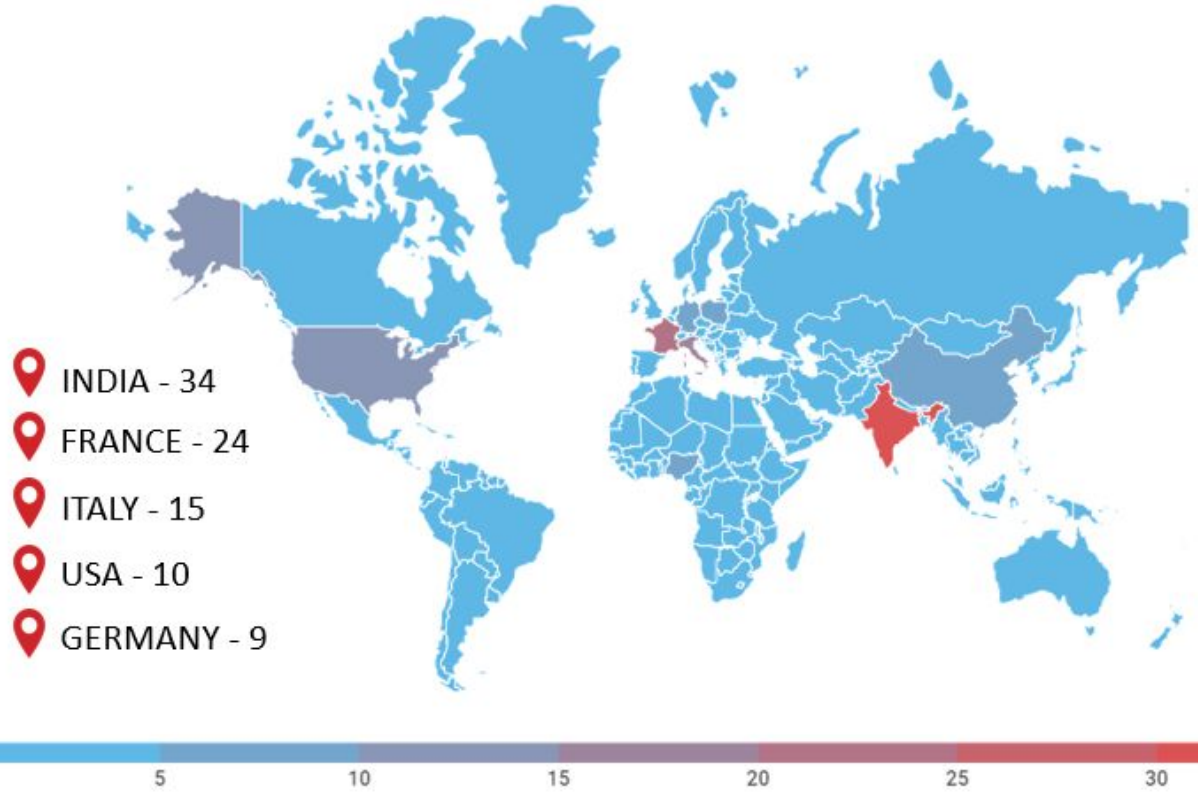
TREX Target stakeholder groups

- Academic and industrial end-users
- Code developers and independent software vendors (ISVs)
- European HPC ecosystem
- Hardware manufacturers
- Communities from EU countries currently developing and advancing their HPC infrastructure and ecosystem
- Centres of Excellence on HPC
- Education system

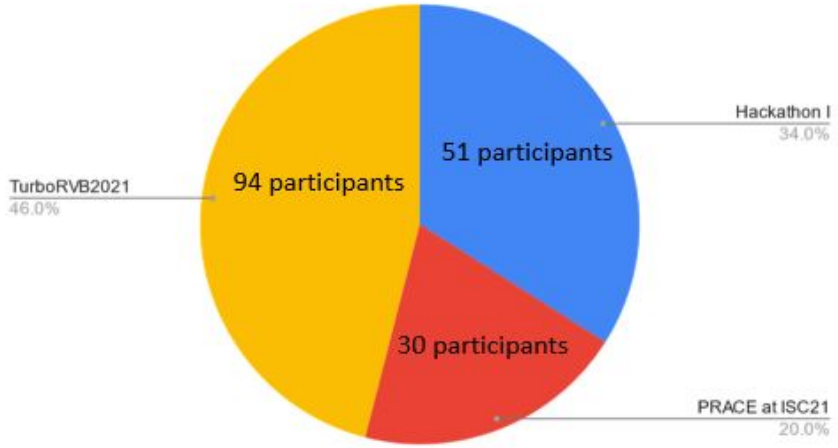
TREX 2021 workshops and schools

Event Participants by Country

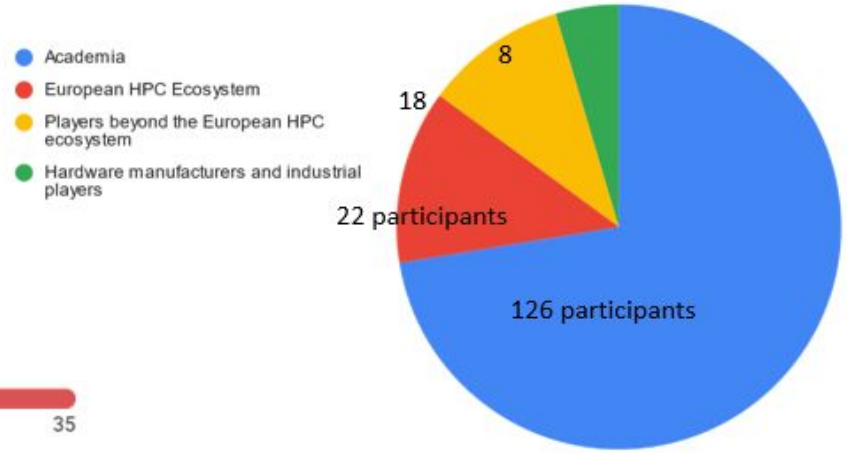
174 total participants coming from
40 countries around the world



Participants by Event



Participants by Stakeholder group



Interfacing strategy within European HPC ecosystem: events

D8.3

Month	Event	TREX contribution
June 2020	Presentation (UT) to **HPC3 Council**	Potential synergies for collaborations on software development, applications, and training were sought
November 2020	Participation (UVSQ) to **Instructor training workshop for HPC CoEs**	Teach and design lessons related to scientific software engineering and HPC applications NB: UVSQ contact point of FocusCoE on training
December 2020	Participation (CNRS/Paris, Megware) to the **Webinar on the interaction with industries and SMEs**	TREX outputs will be an asset to strengthen the European HPC ecosystem due to their potential exploitability in business-oriented projects.
March 2021	Panelist participation (CINECA, CNRS/Toulouse) to **Co-design Workshop for CoEs**	The TREX software strategy was described, which consists in refactoring the performance-critical routines and merging them into the high-performance library of kernels QMCkl, which is developed within WP1 and WP3

Alignment & collaboration with other COEs

D8.3

MAX DRIVING THE EXASCALE TRANSITION

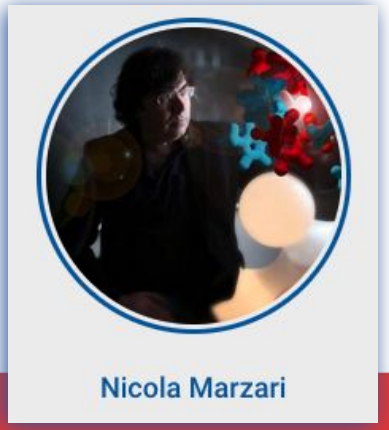
TREX is complementary to MAX in methodology, actual software, and typology of quantum problems

TREX is capitalizing on and enhancing one infrastructural initiative of Max, having adopted the **AiiDA Materials Informatics Framework** for workflow management, data storage, persistence, and provenance

- ➔ AiiDA will be enriched with TREX quantum Monte Carlo codes (**CHAMP, TurboRVB, QMC=CHEM, and NECI**) for quantum calculations at high accuracy.
- ➔ TREX will “bring” to AiiDA other deterministic quantum chemical codes
- ➔ The integration of AiiDa with the **Materials Cloud Archives** will also expose our curated high-level data to the MaX communities.

Joint events/meetings in Oct 2020, July, Oct, Nov 2021

Nicola Marzari member of TREX Advisory Board



D8.3

Alignment & collaboration with other COEs

NOMAD
NOVEL MATERIALS DISCOVERY

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

➔ TREX tutorial lecture (UT) on “Quantum Monte Carlo”planned at the International Summer School on Electronic Structure Theory and Materials Design organized by **Computational Atomic-scale Materials Design** Section at the Technical University of Denmark **(August 2022)**

Interest for adopting a common file format and using the Input/Output TREXIO library (**WP2**)

TREX is connected to the **Performance Optimization and Production CoE** (POP2) through our partner **UVSQ**

UVSQ has been mainly involved in single-core and single-node performance analysis using **MAQAO**

Any improvements brought to the TREX flagship codes and the QMCkl library will directly benefit the quality of analyses and metrics performed in the context of PoP.

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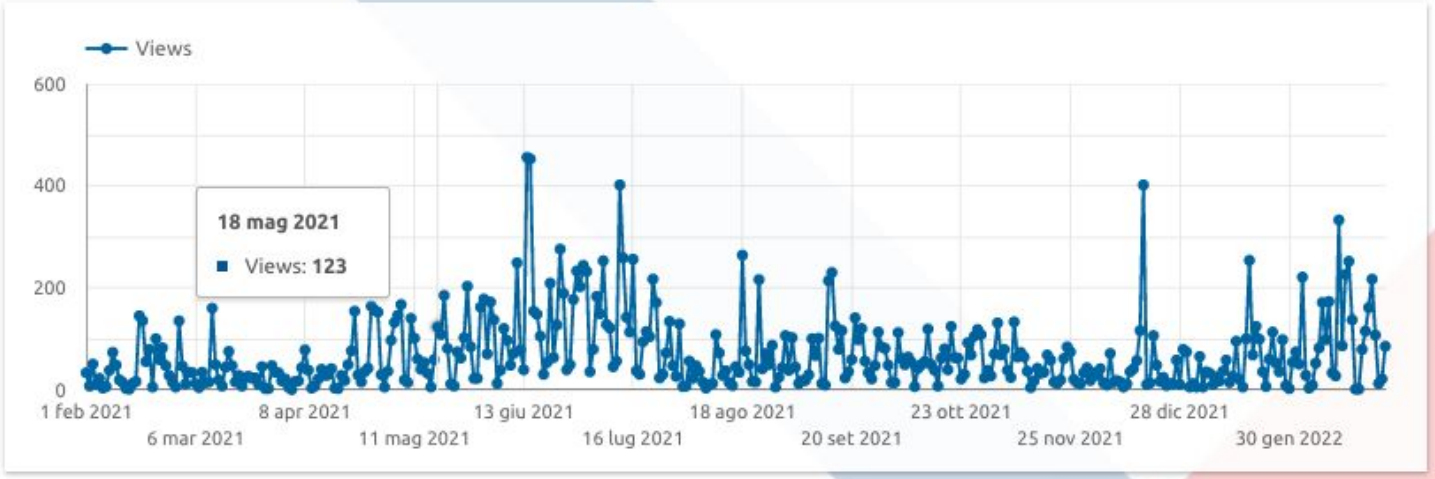
TREX website traffic Feb 2021 - Feb 2022

- **174 participants** in the Main Events (TurboRVB School, Building System Hackathon I, PRACE workshop)
- **101 Subscribers** to our Newsletter



	Page path	Views	Engagement rate	Sessions
1.	/	5.163	62,3%	3.743
2.	/events/trex-e-school-quantum-monte-carlo-turborvb	1.571	49%	1.196
3.	/publications	1.486	54,63%	216
4.	/events	1.325	40,38%	156
5.	/open-positions	1.103	42,17%	351
6.	/events/trex-build-system-hackathon-8-12-nov-2021	938	44,04%	738
7.	/partners/teams	807	55,96%	277
8.	/trex-e-school-quantum-monte-carlo-turborvb-programme	701	49,82%	566
9.	/partners	661	52,99%	134
10.	/about-trex-hpc-centre-excellence-quantum-chemistry	601	40,54%	185
11.	/trex-quantum-chemistry-codes	518	36,14%	166
12.	/trex-e-school-registration	513	65,32%	372

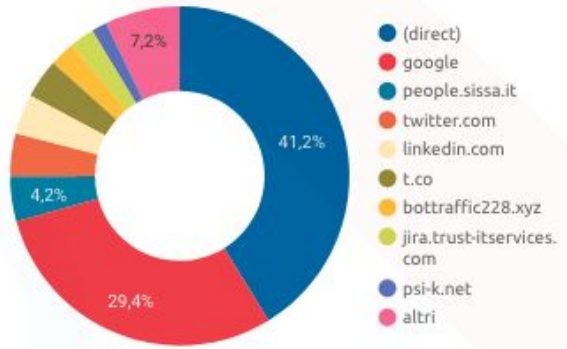
1 - 100 / 538

Views	Sessions
27.002 ↑ 567.0%	11.647 ↑ 486.8%
Active users	**New users**
6.284 ↑ 450.3%	7.842 ↑ 587.3%

Session Duration
452:46:57

Event count	Engagement rate
77.129 ↑ 564.7%	54,99% ↓ -1.4%

Source of traffic



TREX overall engagement: Twitter overview

Overall figures:

- 205 Followers
- 10.031 Profile visits
- 95.765 Tweet Impressions
- 18,1 % Engagement Rate

TREX overall engagement: Linkedin overview

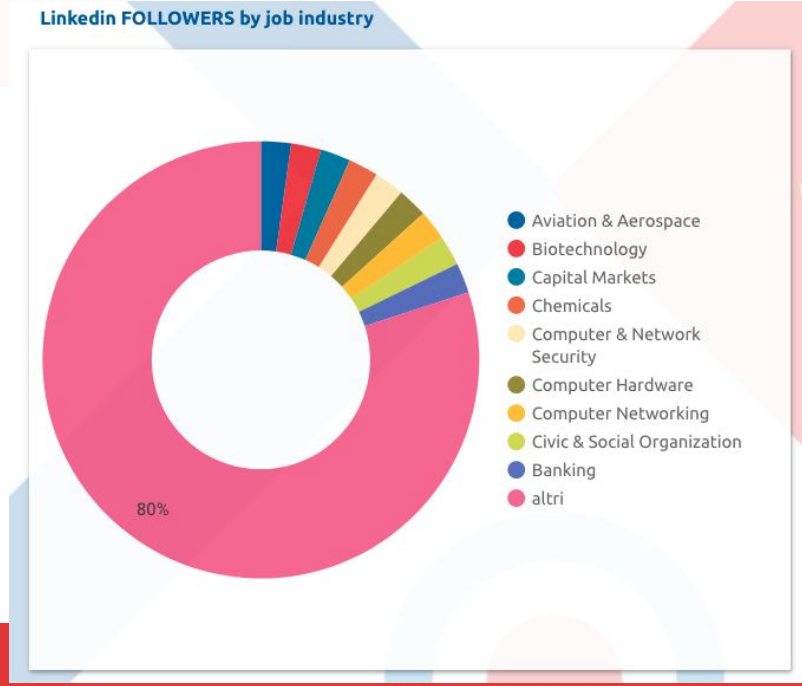
Top locations

	Followers	% of Followers
Pisa Area, Italy	26	10.57%
Bologna Area, Italy	13	5.28%
Paris Area, France	13	5.28%
Amsterdam Area, Netherlands	12	4.88%
London, United Kingdom	9	3.66%
Enschede Area, Netherlands	9	3.66%
Barcelona Area, Spain	9	3.66%
Rome Area, Italy	7	2.85%
Trieste Area, Italy	6	2.44%
San Francisco Bay Area	6	2.44%

Top job functions

	Followers	% of Followers
Research	98	35.38%
Education	43	15.52%
Engineering	34	12.27%
Media and Communication	22	7.94%
Business Development	14	5.05%
Program and Project Management	13	4.69%
Information Technology	11	3.97%
Marketing	10	3.61%
Operations	10	3.61%
Sales	4	1.44%

740 LinkedIn Connections and 336 followers of the TREX page



TREX Communication trends

Targeting Real chemical accuracy at the EXascale

menti.com

2088 9078

TREX Exploitable results

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TREX assets and key exploitable results

According to the Horizon 2020, a result is defined as: *"Any tangible or intangible output of the action, such as data, knowledge and information whatever their form or nature, whether or not they can be protected, which are generated in the action as well as any attached rights, including intellectual property rights".*

D8.4

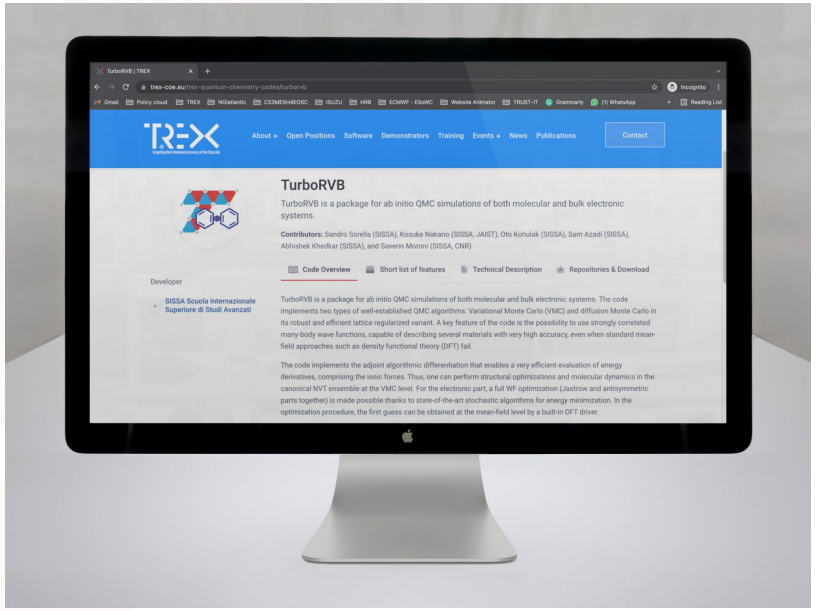
TREX Asset: TREX flagship codes and libraries

Asset name	Type	Main Developer
Quantum Package	Code	CNRS
QMC=Chem	Code	CNRS
CHAMP	Code	UT
TurboRVB	Code	SISSA
GammCor	Code	TUL
NECI	Code	MPG
TREXIO	Library	TREX
QMCkl	Library	TREX

Quantum Package	
Result Type	**Scientific and Technological R&D Result including ICT Software and Digital solution**
Result Contributors	Anthony Scemama (CNRS) As part of TREX: Abdallah Ammar (CNRS), Evgeny Posenitskiy (CNRS), Vijay Gopal Chilkuri (CNRS)
Owners for exploitation	CNRS
Result description	Quantum Package is an electronic structure software focused on wave function methods (configuration interaction) combined with density functional theory. It allows estimating full configuration interaction energies with the CIPSI algorithm, and provides a friendly environment for the development of new methods. The code is available under the GNU AGPL license and has shown a good scalability with up to 20 000 CPU cores.
Target audience	Theoretical chemistry community, quantum simulation of materials community.
Results maturity (TRL)	Individual TRL9: the software has been validated and used on several Tier-0 supercomputers. Multiple critical applications have been published. Integrated TRL3
Current Stage and Next Steps	We have implemented a new algorithm to reduce the memory usage of the program, enabling the simulation of larger systems. We are preparing the next version of the code where we will integrate the use of the TREXIO library for reading/writing the wave function parameters and removing an I/O bottleneck.
Do you already have customers for this result?	Yes – research groups around the world use Quantum Package to solve problems of topical interest in quantum chemistry and physics.

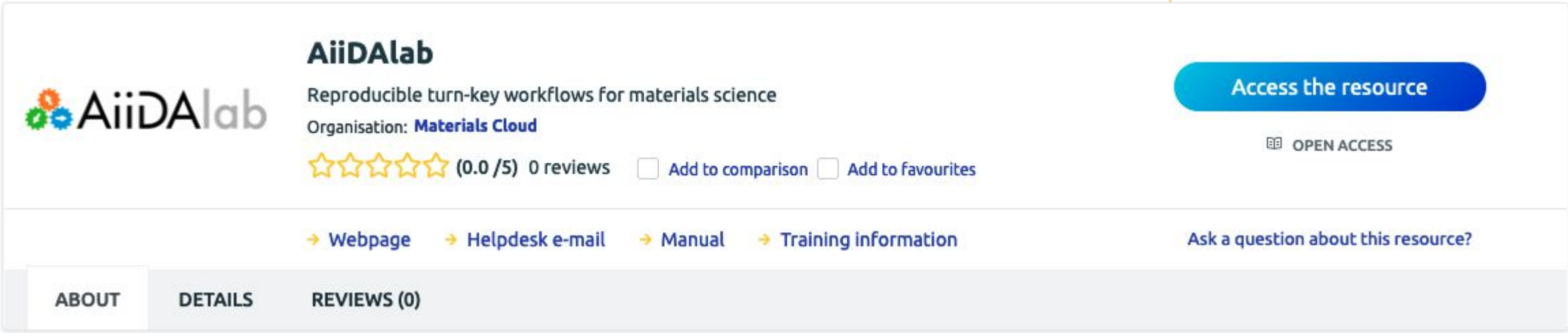
D8.4

Template filled in for all TREX codes and TREX Libraries, used to present information online at https://trex-coe.eu/trex-quantum-chemistry-codes



Exploitation plans: what about the EOSC Marketplace?

EUROPEAN OPEN SCIENCE CLOUD



https://marketplace.eosc-portal.eu/services/aiida-lab

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TREX Support Centre: ideas & discussion

Fabio Affinito, CINECA

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TREX publications

21 publications released
6 also on zenodo

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

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POSTER
TREX Targeting REal Accuracy at eXascale
21 OCT 2021
Affinito, Fabio
In order to compete in the demanding rush in high-precision quantum chemical simulation methods, the TREX Center of Excellence (CoE) federates European scientists, High Performance Computing (HPC) stakeholders, and SMEs to develop and apply high-performance so.. Read more

PRESENTATION
TREX : an innovative view of HPC usage applied to Quantum Monte Carlo simulations
02 JUL 2021
Scemama, Anthony; de Oliveira Castro, Pablo; Valensi, Cedric; Jalby, William
TREX : an innovative view of HPC usage applied to Quantum Monte Carlo simulations The TREX[1] European Center of Excellence focuses on high accur.. Read more

PROJECT ARTICLE
Spin-adapted selected configuration interaction in a determinant basis
03 JUN 2021
Chilkuri, Vijay Gopal; Applencourt, Thomas; Gasperich, Kevin; Loos, Pierre-Francois; Scemama, Anthony
Selected configuration interaction (SCI) methods, when complemented with a second-order perturbative correction, provide near full configuration interaction (FCI) quality energies with only a small fraction of the Slater determinants of the FCI space. However,.. Read more

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Spin-adapted selected configuration interaction in a determinant basis
Chilkuri, Vijay Gopal; Applencourt, Thomas; Gasperich, Kevin; Loos, Pierre-Francois; Scemama, Anthony;
Selected configuration interaction (SCI) methods, when complemented with a second-order perturbative correction, provide near full configuration interaction (FCI) quality energies with only a small fraction of the Slater determinants of the FCI space. However, a selection criterion based on determin
Uploaded on June 3, 2021

April 22, 2021 (v1) | Presentation | Open Access — View
Library development within TREX
Anthony Scemama;
Presentation of: - TREX - QMCkl - TREXIO
Uploaded on April 22, 2021

April 16, 2021 (v1) | Presentation | Open Access — View
Guidelines for improving the performance of computer programs
Anthony Scemama;
Webinar organized by Institut Chimie Radicalaire & Centre de Calcul Intensif Aix-Marseille. The technological evolution of

Community

Targeting Real chemical accuracy at the EXascale

TREX - Targeting Real chemical accuracy at the EXascale

TREX, Targeting Real chemical accuracy at the EXascale, is the European Centre of Excellence (CoE) in Exascale Computing **federating European scientists, High Performance Computing (HPC) stakeholders, and SMEs to develop and apply high-performance software solutions for quantum mechanical simulations at the exascale.** The final goal of the project is to develop a set of flagship **Quantum Monte Carlo codes**, able to exploit the capabilities of the recent exascale computers at its highest.

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

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TREX
Curation policy:
This collection contains material produced by TREX project partners in the context of the project.
Created:
April 22, 2021
Harvesting API:
OAI-PMH Interface

Upcoming events

Event	Date	Location	Classification
EuroHPC Summit week 2022/PRACEdays22 (EHPCSW 2022)	22-24 Mar 2022	Paris, France	3rd-party event
QMC Hands-on Summer Workshop	20-23 Jun 2022	Mojmírovce, Slovakia	TREX organised event
First TREX School on QMC with TurboRVB	4-8 Jul 2022	Trieste, Italy	TREX organised event
TERATEC FORUM 2022 (TBC)	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 (TBC)	22-25 Aug 2022	Paris, France	3rd-party event

Plans for the next 6 months

March: Promotion of the input/output library (TREXIO)

- March: New pages showing the alignment & collaboration with other COEs
- March: clean IPs to fine tune source of traffic
- April/May: new pages dedicated to the TREX demonstrators
- April/May: training and use support materials to be added to the code pages

- Define engagement actions for TREX scientific user communities, developers, and scientists in materials sciences → *via the Demonstrators?*
- Finalisation of the exploitation plans
- *TREX flagship codes webinar series?*

WP7 KPIs

KPI	KPI description	Target	M18
KPI 7.1	Community database	50 (M12), 150 (M24), 300 (M36)	200 website registrations
KPI 7.2	Social media coverage targets	Twitter (M36) 100 tweets >100 followers	205 followers 162 Tweet
		LinkedIn 100 connections	405 Connection (profile) 336 Connection (project) 741 Total connections
		30 mentions on 30 external social media channels	105 mentions
KPI 7.3	Website targets	Number of session	13.820 Session
		Downloads of outputs	*Code leaders
		Site bounce rates	49.30% Bounce Rate
KPI 7.4	Transfer of research results, service offers, and event related targets	250 participants (M36)	174 Participants
		30 stakeholders reached on webinars (M36)	In progress - webinars will be part of M19-M36 initiatives
KPI 7.5	Videos production targets	3 videos (M36)	13 Videos
		200 YTC views	826 YouTube Views
KPI 7.6	Impact of social networking and viral marketing	10 TREX applications of industrial/technological interest	*Megware or UT
		4 other quantum chemical packages integrating TREX codes	*Jan Beerens/Claudia(UT)
		50 end-users exploiting QMC codes	*Code leaders
		10 occasions, where TREX SW is used as teaching tools	10 occasions/events
		1 FInal Blueprint, reaching 200 community members	In progress
KPI 7.7	Impact of media outreach	10 newsletter (M36)	3 Newsletter
		12 articles by specialised/general media	14 Articles
		6 content pieces published on external channels	5 News pieces