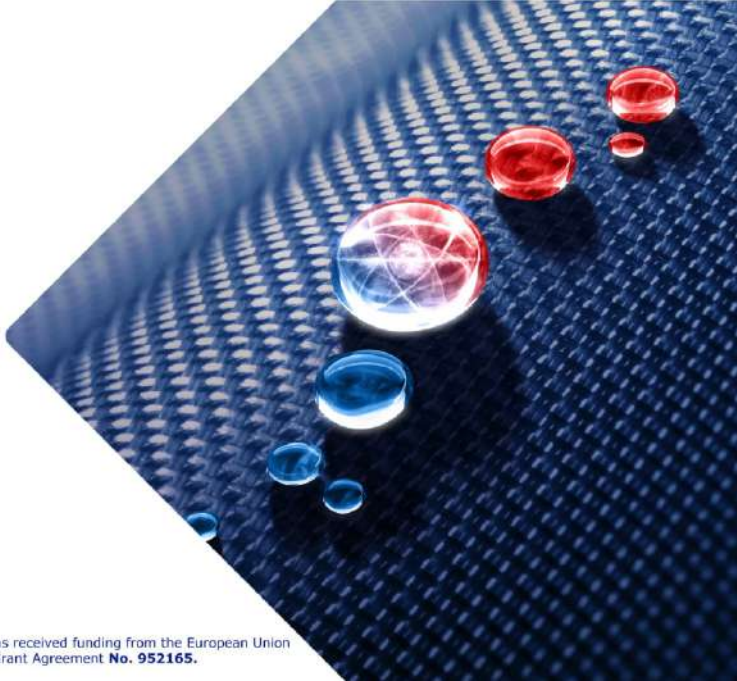
Targeting Real chemical accuracy at the EXascale

Few words about TREX Center of Excellence

Claudia Filippi

University of Twente, The Netherlands



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. 952165.**


European Commission | CORDIS EU research results
English EN
Search
HOME THEMATIC PACKS PODCASTS & NEWS PROJECTS & RESULTS ABOUT US SEARCH
LOG IN
HORIZON 2020
Targeting Real chemical accuracy at the EXascale
Fact Sheet
Results
News & Multimedia
Project description
Complex quantum molecular simulations of unprecedented speed and accuracy
Computers and the rapid mathematical calculations they are able to perform, which would take human beings years to accomplish, have provided the fuel to power innovation. High-performance computing (HPC) and high-throughput computing (HTC) have enabled us to simulate large-scale complex processes and analyse tremendous amounts of data, benefitting 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 EU-funded TREX project is developing a platform that combines the upcoming exascale HPC and HTC architectures for stochastic quantum chemical simulations of unprecedented accuracy. The software and services will be designed for ease of use to ensure widespread utilisation, spurring a new age of discovery in molecular simulations.
Show the project objective
Project Information
TREX
Grant agreement ID: 952165
DOI
10.3030/952165
Start date
1 October 2020
End date
30 September 2023
Funded under
EXCELLENT SCIENCE - Research Infrastructures
Total cost
€ 4 998 847,50
EU contribution
€ 4 998 847,50
Coordinated by
UNIVERSITEIT TWENTE
Netherlands

TREX - Targeting Real chemical accuracy at the EXascale

Focus → quantum Monte Carlo (QMC) methods

- Very accurate methods (molecules and solids)
- Massively parallelisable: multiple QMC "trajectories"
- Very CPU intensive → "compute-hungry" method!
- Still under development: we need to run and develop code

Objective → make codes ready for exascale systems

How → provide libraries instead of re-writing codes!

- QMCkl : library for high-performance QMC → HPC
- TREXIO : library for exchanging info between codes → HTC

Scientists in quantum chemistry, physics, and machine learning

+ Software and HPC experts + Tech and communication SMEs

+ Representative of user communities

TREX HPC platform of interoperable software

- The libraries QMCkl and TREXIO
- TREX codes refactored and modularized to use these libraries

  CHAMP, QMC=Chem, TurboRVB, NECI

  Quantum Package, GammCor
- Machine learning tools integrated in our workflows

  → AiiDA for workflow managment/HTC

- TREX website : `https://trex-coe.eu`
- TREX repository : `https://github.com/TREX-CoE`

Acknowledgments