

Introduction TREX Center of Excellence

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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.**



TREX - Center of Excellence in Exascale Computing



Targeting Real chemical accuracy at the EXascale

Fact Sheet News & Multimedia

2020

Project description

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Complex quantum molecular simulations of unprecedented speed and accuracy

Computer and the rapid mathematical calculations they are able to perform, which would take human beings years to accomplish, huwe provided the take to power invovation. Http-performance computing (HPC) and high-throughput computing (HTC) have enabled us to simulate large-scale complex processes and analysis termendous amounts of data, benefitting applications ranging from climate research and daug discovery to material design. Emerging axecate computers will make the best even better, 50 times taket than today's most powerful supercomputers. The EU-funded TREX project is developing a platform that combines the upcoming exacele HTCP and HTC artifectures for storabid quantum channels aimutations of upprecedented accuracy. The software and services will be designed for ease of use to ensure widespread utilisation, spuring a new age of discovery in molecular simulations.

roject Information		
TREX Grant agreement ID: 952165		
Status Ongoing project		
Start date 1 October 2020	End date 30 September 2023	
Funded under H2020-EU.1.4.1.3. Overall budget € 4 998 847,50		
EU contribution € 4 998 847,50	U	
Coordinated by UNIVERSITEIT TWENTE		

Hide the project objective



- Started in October 2020
- [Focus] \rightarrow High-accuracy quantum chemical approaches
 - In particular, quantum Monte Carlo (QMC) methods
 - Massively parallelisable methods: multiple QMC "trajectories"
 - Small I/O and memory, (often) little communication
- Objective \rightarrow make codes ready for exascale systems
- How \rightarrow provide libraries instead of re-writing codes!
 - One library for high-performance QMC (QMCkl)
 - One library for exchanging info between codes (TREXIO)



TREX CoE: Partners



Scientists in quantum chemistry, physics, and machine learning + Software and HPC experts + Tech and communication SMEs + Representative of user communities



Quantum Monte Carlo

 \rightarrow Stochastic simulation of the quantum interacting problem

Very accurate calculations for medium-large molecules and periodic systems!



Casula and Sorella (2013)

CPU intensive but can scale to massive parallelism



Ease in parallelization of QMC is not sufficient for accurate results

Recent methodological advances \rightarrow new prospects

- Efficient computation of analytical energy derivatives + optimization tools
 - ightarrow QMC "internally consistent" method

with geometries and wave functions determined in QMC

- Truly exploit freedom of choice of wave function $\Psi(r_1, \ldots, r_N)$ \rightarrow development of new functional forms (geminals, FermiNet ...)



Software model \rightarrow HPC platform of interoperable codes/libraries

- QMCkI high-performance (CPU and GPU) library of QMC kernels
- TREXIO library to exchange wave function data
 - \rightarrow Easy use of TREX + other codes (GAMESS, PySCF, Gaussian ...) in a pipeline
- TREX codes refactored and modularized to use these libraries
- Machine learning tools integrated in our workflows



 \rightarrow SAiiDA Informatics Framework adopted for workflow managment/HTC



- Real-space QMC: 🖤 CHAMP, 🞄 QMC=Chem, 🌌 TurboRVB
- Full configuration interaction QMC: Section NECI
- Deterministic quantum chemical codes: 🧖 Quantum Package, 🖼 GammCor





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- Full configuration interaction QMC: Section NECI
- Deterministic quantum chemical codes: 🥺 Quantum Package, 🛤 GammCor
- Machine learning: QMMLPACK
- Performance and optimization tools: MARAO MAQAO, Kincol Verificarlo
- Software for cloud-style access to HPC resources: MEGWARE







- TREX website : https://trex-coe.eu
- Training :

 $\verb+https://trex-coe.eu/trex-training-and-educational-programme$

TREX repository : https://github.com/TREX-CoE





- Presentation of codes and TREXIO library
- Presentation of examples of use of codes