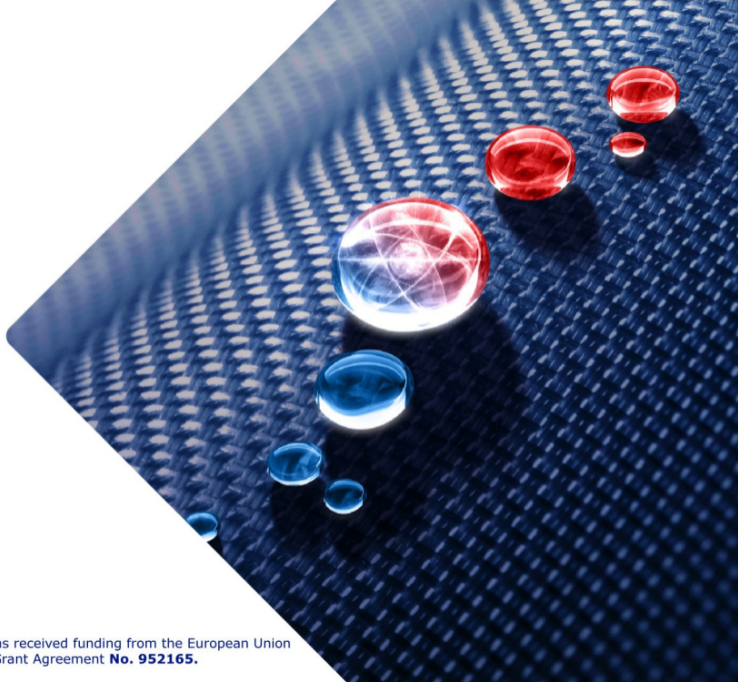




Few words TREX Center of Excellence

Coordinator: Claudia Filippi

University of Twente, The Netherlands



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



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!

- **QMCKI** : 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 Hackathon II at Université de Versailles-Saint-Quentin-en-Yvelines (March 2022)

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 management/HTC

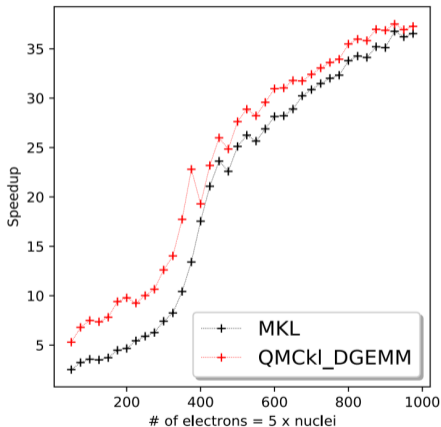
QMCKl → Main kernels of QMC calculations

Example: Jastrow factor

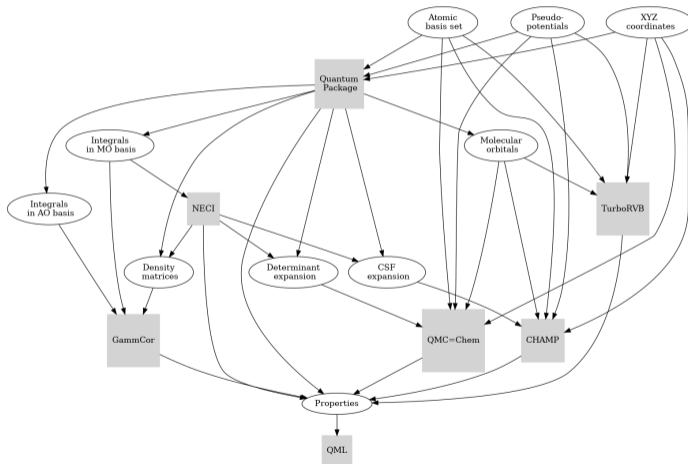
Extracted from Ψ CHAMP code

Optimization guided by  MAQAO

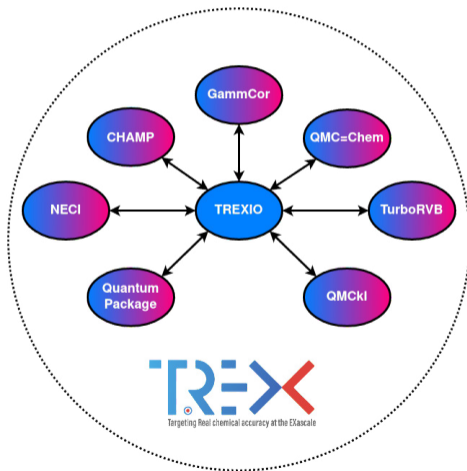
Analysis of code binary generated by compiler

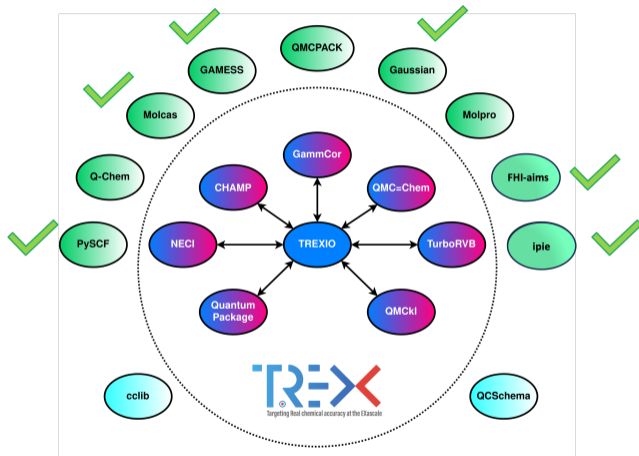


Original situation within TREX



Current status within TREX





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