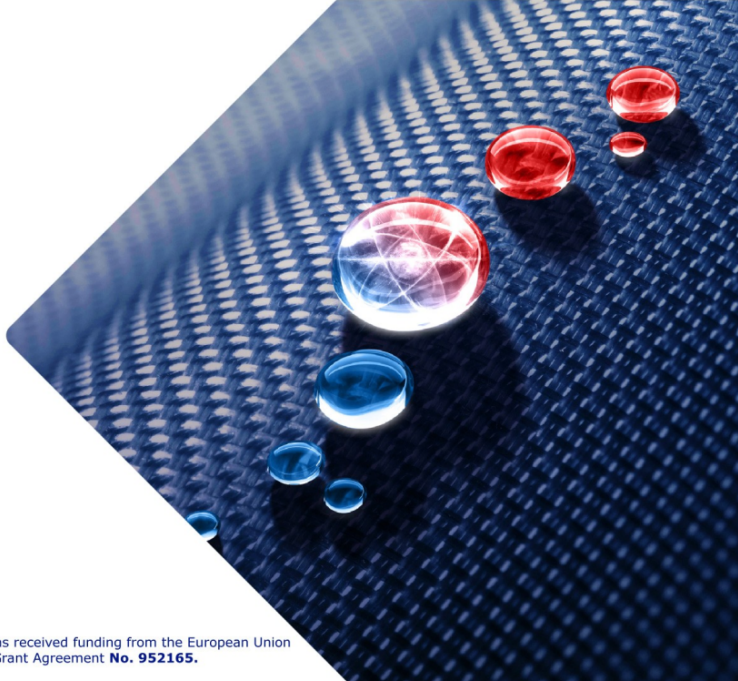
Targeting Real chemical accuracy at the EXascale

Few words TREX Center of Excellence



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TREX - Center of Excellence in Exascale Computing

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 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 managment/HTC

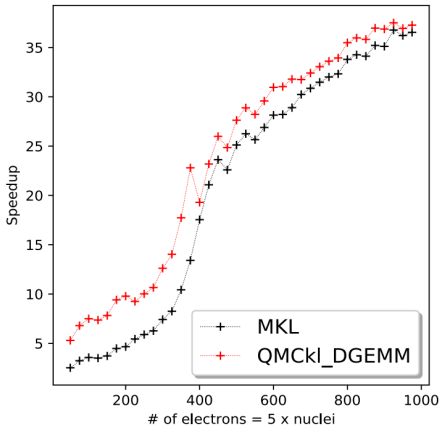
QMCkl → Main kernels of QMC calculations

Example: Jastrow factor

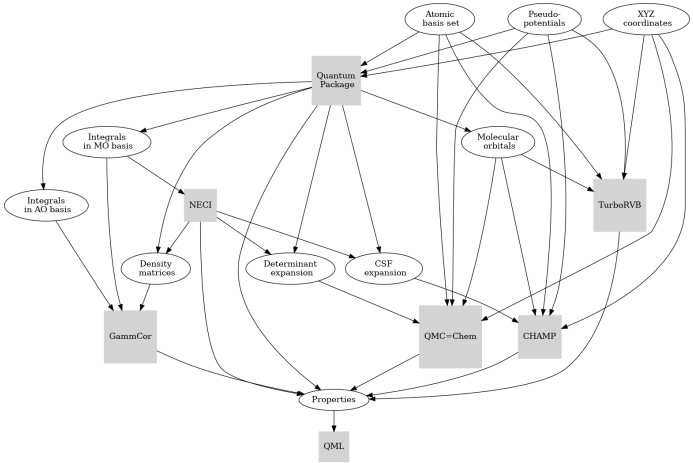
Extracted from CHAMP code

Optimization guided by MAQAO

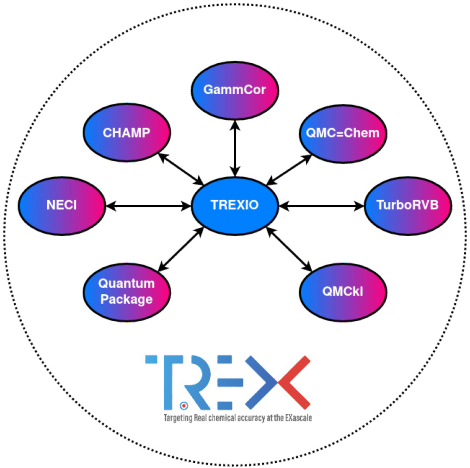
Analysis of code binary generated by compiler



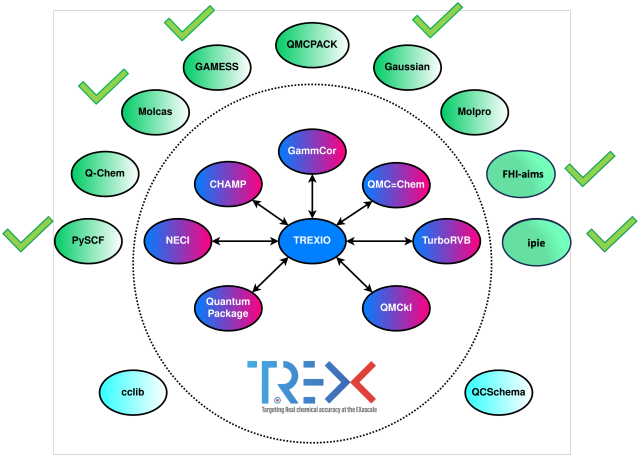
Original situation within TREX



Current status within TREX



TREXIO: status



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