Computers can perform extremely fast calculations which would take human beings years to accomplish, accelerating innovation to unprecedented levels. High-performance computing (HPC) and high-throughput computing (HTC) have enabled us to simulate large-scale complex processes and analyze 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 TREX Center of Excellence (CoE) federates European scientists, HPC stakeholders and SMEs to develop and apply high-performance software solutions for high-accuracy quantum mechanical simulations at the exascale.

TREX

Targeting Real chemical accuracy at the EXascale

Enabling the community codes for stochastic quantum chemical simulations at the exascale.

TREX Main Outcomes

Co-design of computational kernels of flagship quantum Monte Carlo (QMC) codes with efficient scalable algorithms for HPC applications of chemical accuracy.

Rational design of an ecosystem of highly scalable, optimized and interoperable QMC codes.

Robust management of complex scalable QMC workflows in high-throughput calculations.

Foster wider access, usage and uptake of knowledge in HPC and quantum chemical simulations with direct involvement of user communities via demonstrators.

TREX Codes

TurboRVB

TurboRVB is a package for ab initio quantum Monte Carlo simulations of both molecular and bulk electronic systems

CHAMP

The Cornell-Holland Ab-initio Materials Package (CHAMP) is a quantum Monte Carlo package for electronic structure calculations of molecular systems

QMC=Chem

QMC=Chem is a quantum Monte Carlo package for electronic structure calculations of molecular systems

TREXIO

The TREXIO library defines a standard format for storing wave function parameters, together with a C-compatible API such that it can be easily used in any programming language

NECI

NECI implements the configurations interaction quantum Monte Carlo method to simulate molecular systems containing many electrons and to obtain their properties with chemicals accuracy, including energy spectra, reaction pathways, etc.

Quantum Package

Quantum Package is an electronic structure software focused on wave function methods (configuration interaction) combined with density functional theory

GAMMCOR

GAMMCOR is an advanced quantum chemical software package for the accurate computation of weak interactions in supramolecular systems

QMCkl

The QMCkl library aims at providing a high-performance implementation of the main kernels of quantum Monte Carlo methods

TREX Consortium

TREX is a committed, competent and complementary consortium of 12 partners from 7 European countries led by the University of Twente

University of Twente. · CNRS · SISSA (ma per seguir virtute e canoscenza) · CINECA · Max-Planck-Gesellschaft · Université de Versailles St-Quentin-en-Yvelines / Université Paris-Saclay · MEGWARE · Slovenská akadémia vied · Politechnika Łódzka · Luxembourg Institute of Science and Technology (LIST) · Trust-IT Services communicating to markets · Universität Konstanz

Key figures

Start **01 OCT 2020** End **31 MAR 2024**

Join the TREX Community

TREX: Targeting Real Chemical Accuracy at the Exascale project has received funding from the European Union Horizon 2020 research and innovation programme under Grant Agreement No. 952165.

www.trex-coe.eu · @trex_eu · TREX Project · TREX Channel