TREX

Targeting Real chemical accuracy at the EXascale

Enabling the community codes for stochastic quantum chemical simulations

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 TREX Center of Excellence (CoE) federates European scientists, High Performance Computing (HPC) stakeholders, and SMEs to develop and apply high-performance software solutions for quantum mechanical simulations at the exascale.

TREX Main Outcomes

Co-design of computational kernels of flagship QMC codes with efficient scalable algorithms for HPC applications.

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 via direct involvement of present and potential user communities via demonstrators.

TREX Codes

TurboRVB

TurboRVB is a package for ab initio QMC 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 full configuration interaction quantum Monte Carlo method, a particularly efficient formulation of the full configuration interaction, which simulates molecular systems containing tens of electrons and obtains their properties with chemical accuracy, including energy spectra, density matrices, 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 open-source program licensed under GNU GPLv3

QMCkl

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

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TREX Consortium

The **TREX consortium** is committed to building an efficient and state-of-the-art framework in HPC and exascale computing by developing an **integrated software platform**.

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Key figures

Start **01 OCT 2020** End **30 SEP 2023**

Join the TREX Community

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