TREX

Targeting Real chemical accuracy at the EXascale

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

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 software for quantum mechanical simulations

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 offer for INDUSTRY

Whether it comes to lighter, yet stronger materials for aerospace applications or whether it is the design of new catalysts used in energy storage and conversion: digitalization and the development of advanced novel materials are at the center of innovation across many industries.

With the help of accurate chemical simulations and machine-learning models, the physical properties of a new material, for example, its thermal conductivity, can be determined even before it is first synthesized, thus saving cost-intensive lab hours and accelerating innovation.

Empowering European microprocessors' industry: TREX & Sipearl

SIPEARL

Quantum chemistry is a critical foundational science for the future of European technology. The workloads that TREX is addressing will lead to important practical applications such as development of catalysts for sustainable fuel production. Developing these codes on the European HPC Microprocessor, designed by SiPearl, as well as co-designing hardware & software with them will be an important step in advancing research across European technologies to drive the growth of European Industry.
TREX is also joining forces with SIPEARL and ATOS in the EMOPASS project, use QMCKL and TREX applications to test Sipearl processors.

With its optimized codes and workflows, also thanks to the use of MAQAO performance analysis and optimization framework, TREX not only facilitates the use of chemical simulations in many domains, but also serves as a valuable guidance to the European High-Performance Computing industry that can tailor the next generation of supercomputers even more towards the needs of QMC applications.

MAQAO

UNIVERSITY OF TWENTE. · cnrs · SISSA · CINECA · KTH · UNIVERSITÉ DE VERSAILLES ST-QUENTIN-EN-YVELINES · MEGWARE · SAV · Universität Konstanz · Trust-IT Services

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 Channel · TREX Project