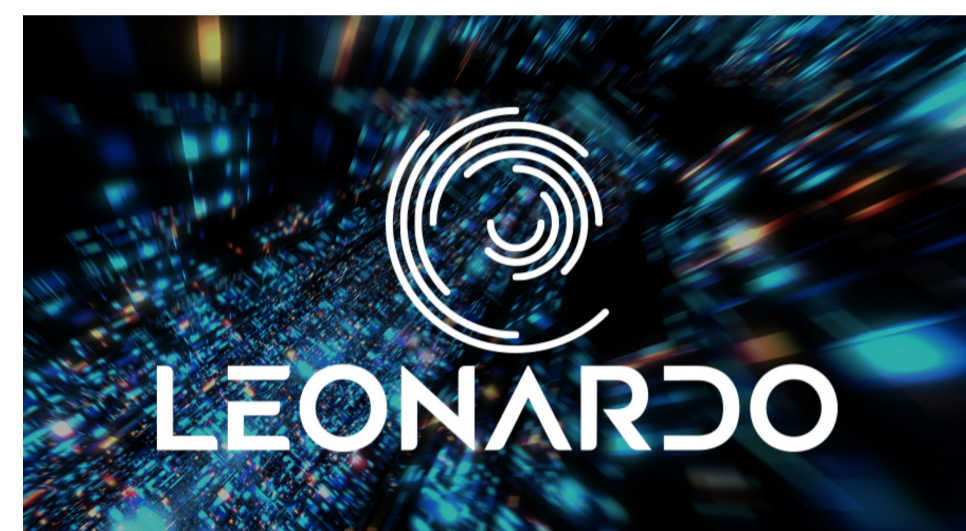
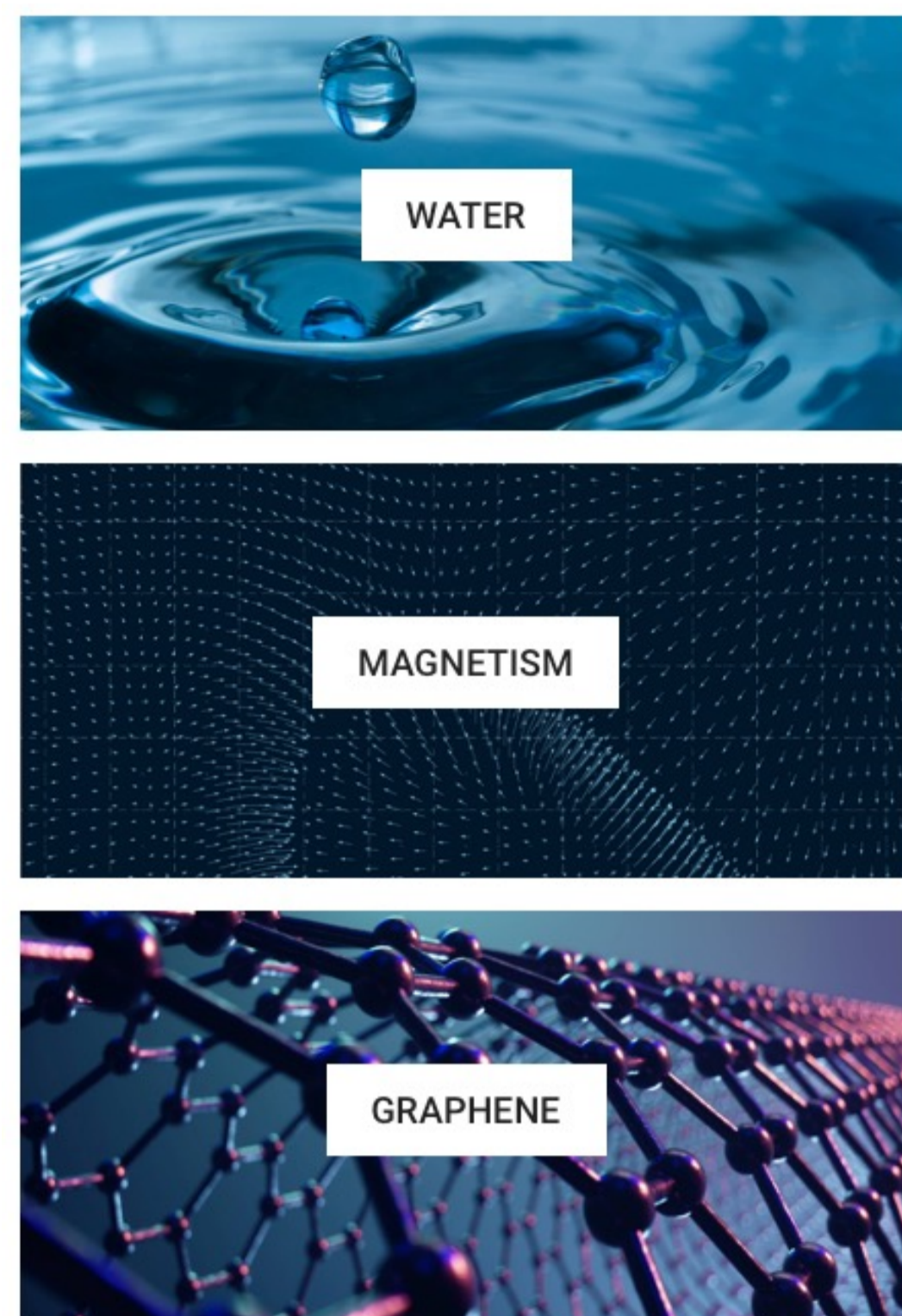


# TREX Targeting REal Accuracy at eXascale



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In order to compete in the demanding rush in **high-precision quantum chemical simulation methods**, 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**. The final goal of the project is to develop a set of flagship **Quantum Monte Carlo codes**, able to exploit the capabilities of the recent exascale computers at its highest.



Next generation of supercomputers will be able to perform up to 1 Exaflop/s ( $10^{18}$  operations per second), running on parallel on tens of thousands of cores. The two first pre-Exascale systems, financed by the EuroHPC JU, LUMI in Finland and Leonardo in Italy will be installed at the end of 2021.

Quantum Montecarlo methods can leverage this computational power thanks to the intrinsic parallelism of the QMC trajectories.

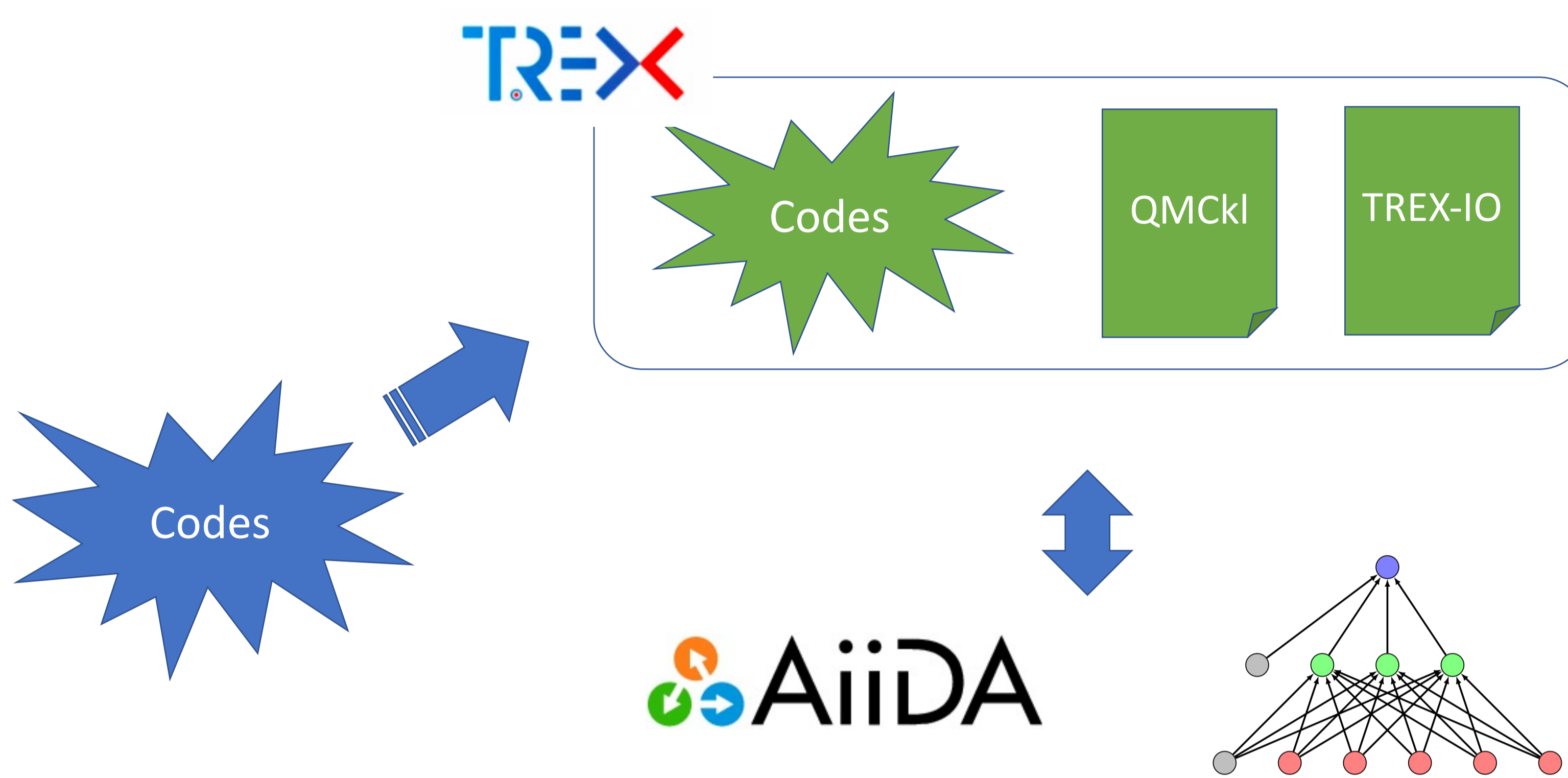
The TREX Center of Excellence joins the forces and the expertises of the experts in the fields of quantum chemistry with the skills of computational scientists and HPC experts with the aim is to guide the evolution of the QMC codes in order increase their efficiency.

## TREX strategy

Instead of rewriting the codes, our strategy looks at the extract the common parts in order to build-up specialized libraries:

- **TREX-IO**, to exchange information and data between the TREX codes and to make possible to build complex workflows (High-Throughput calculations)
- **QMCKI**, a library of high-performance tuned kernels whose use is common to all the TREX codes, to keep the pace of the evolution of HPC systems

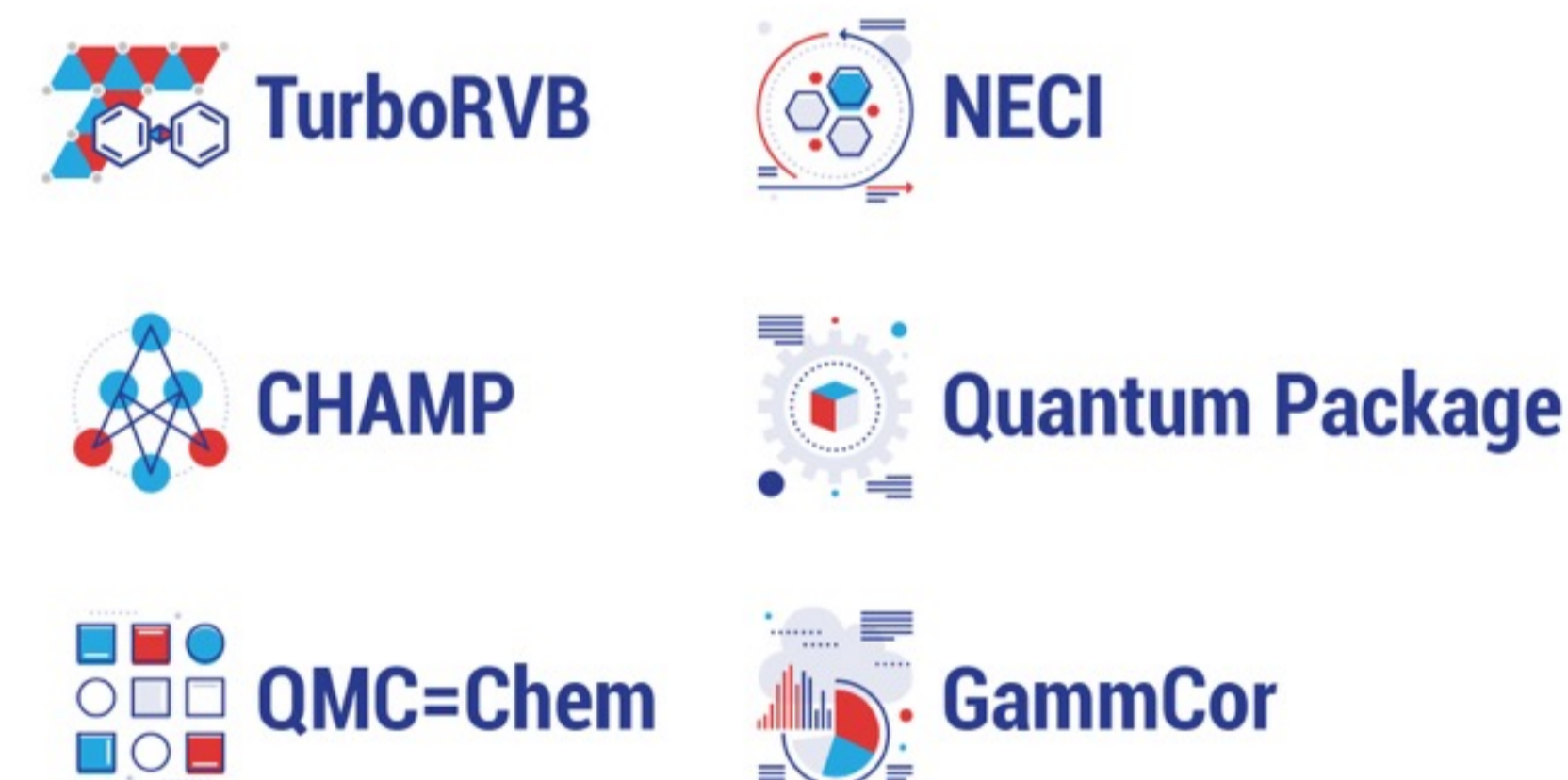
The refactored codes with the TREX libraries will be part of an ecosystem enabling High-Throughput and automated calculations and AI workflows, thanks to the AiiDA framework.



## TREX partners



## TREX codes



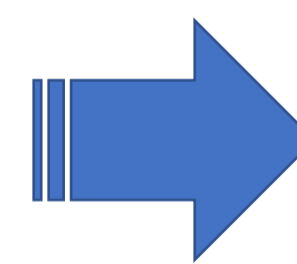
## QMCKI

This library will contain the main kernels of the QMC methods, whose implementation will be designed side by side by domain and HPC experts in order to obtain the best solution both from the technological and the scientific side. It will contain multiple implementations, designed for different HPC architectures, different problem sizes and different required accuracies.



- ✓ **Documentation** version: human-readable, not the most efficient
- ✓ **High performance** version: not human-readable, but tuned for the most possible efficiency

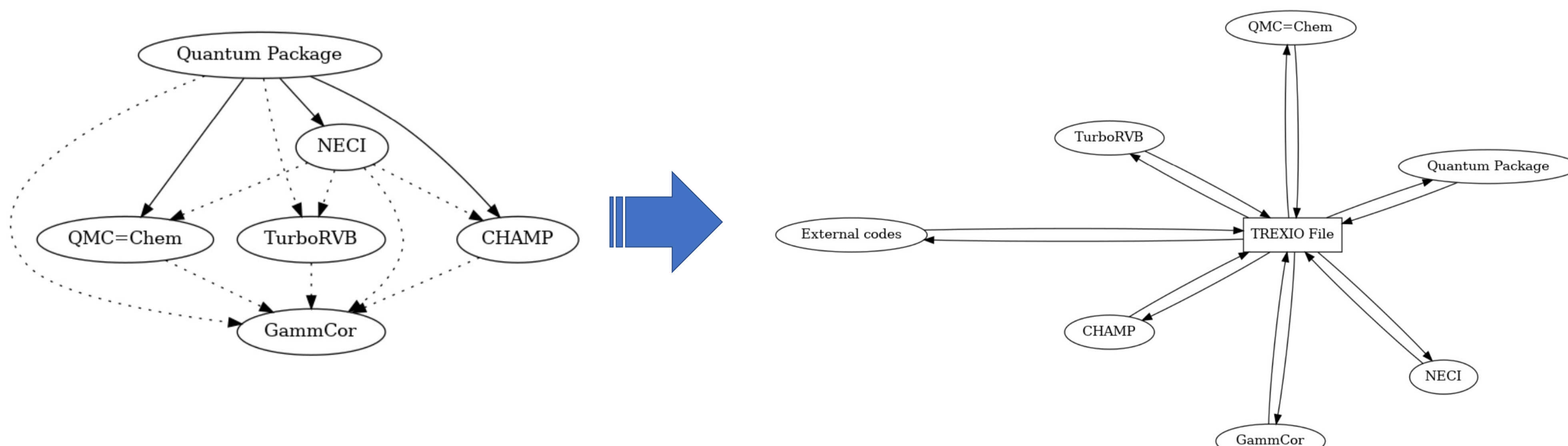
Both versions share the same APIs  
Containing both CPU and GPU versions of the kernels



- ✓ Scientists/Code developers can develop using an easy and human-readable language (**DSL**), not losing the control of their code
- ✓ Aspects related to the tuning to HPC architectures are completely separated and transparent to the code developers (**separation of concerns**)
- ✓ Better **re-use** of optimization effort among the community

## TREX-IO

- ✓ Set of APIs that can be called from the codes to read and write wave functions.
- ✓ Based on HDF5, a portable and efficient I/O format.
- ✓ All files written within this library are self-contained with all relevant information (normalization, parameters, etc.).
- ✓ TREX-IO permits the interoperability of the codes and to build complex high-throughput workflows.



## Links:

- TREX website <https://trex-coe.eu>
- TREXIO <https://github.com/trex-coe/trexio>
- TREX QMCKI <https://github.com/trex-coe/qmcki>
- QMCKI Documentation <https://trex-coe.github.io/qmcki>

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