

## **Libheric: Heterogeneously Accelerated Electron Repulsion Integral Computation**

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The evaluation of four-center electron repulsion integral (ERI) quartets is a fundamental building block of quantum chemistry codes such as CP2K. Accordingly, many algorithms have been developed to reduce the computational complexity of computing ERI quartets (Rys-Quadrature, Obara-Saika, McMurchie-Davidson), resulting in several software libraries that implement these algorithms on modern hardware (Libint, LibintX, Libcint, LibERI, etc.). However, the current ERI library landscape only targets CPU and GPU platforms, even though projects using FPGAs (SorcERI, SERI) and AI-Engines (ERI-AIE) have recently claimed to compute ERIs in a more energy efficient manner. Still, the integration of these novel hardware accelerators into proper quantum chemistry codes remains open.

For this, we present *libheric* and its integration into CP2K. *libheric* provides a hardware accelerator agnostic interface to CP2K by transparently offloading the ERIs to the available accelerators. A CP2K user only has to specify the available hardware accelerators in a simulation input file.

The implementation in CP2K is a complete rewrite of the already existing HFX codepath, which only uses Libint without the vectorization and early-contraction features. *libheric* enables both features for better CPU utilization, and provides GPU acceleration via *libintX*, FPGA acceleration via SERI, and AI-Engine acceleration via ERI-AIE. Additionally, the ERI compression code now leverages PERNIX for AVX2/AVX512 accelerated (de-)compression of integrals, and the computation is now properly screened on the sparsity pattern of the density matrix.

Overall, *libheric* is an ERI library that unifies the interface of existing ERI libraries without sacrificing their performance; all for a seamless integration into quantum chemistry applications. It is an example of true heterogeneous hardware acceleration by bringing novel hardware architectures into the mix.