ID de Contribution: **13** Type: **Non spécifié**

Work on the accelerated calculation of electron repulsion integrals on FPGAs using oneAPI

mercredi 6 juillet 2022 09:30 (30 minutes)

The calculation of electron repulsion integrals (ERIs) is a major bottleneck in quantum chemistry applications. In this work the accelerated calculation of ERIs is developed on Intel Stratix 10 GX 2800 FPGAs by using oneAPI as the high-level synthesis (HLS) tools. To maximize the performance the arrays for intermediate results are carefully designed by taking advantage of the FPGA local memory for parallel data accesses. Via template arguments, multiple different kernel variants for different angular momenta of the input electrons get generated, which allows to fully unroll inner loops with recursive dependencies. Our FPGA kernels for ERIs of high angular momenta outperform the libint library on a compute node with 2 CPU sockets by about 4x. A performance model is established to explain the measured FPGA performance.

Auteur principal: Dr WU, Xin (Paderborn Center for Parallel Computing, Paderborn University)

Orateur: Dr WU, Xin (Paderborn Center for Parallel Computing, Paderborn University)