**Enabling massively parallel relativistic quantum chemistry via ExaTENSOR library**Dmitry Liakh, Luuk Visscher, Hans Jorgen Jensen, Andre Gomes

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**Abstract**

As part of the OLCF Center for Accelerated Application Readiness (CAAR) project, the applicability of the coupled-cluster module of the DIRAC quantum chemistry software is extended to much larger molecular systems with heavy chemical elements. This is done via offloading all numerically expensive computations, namely tensor contractions, to a massively parallel standalone library, ExaTENSOR (OLCF software), capable of executing those operations on GPU-based HPC systems, like Summit and Titan. Additionally, to achieve portability across other HPC architectures, the ExaTENSOR library is designed as a virtual processor that processes tensor instructions and fully encapsulates complex hardware of the underlying HPC system. This results in a separation of the tensor algorithm expression (user level) from its actual execution (virtual processor level) , thus hiding the hardware complexity from the domain scientist. Underneath, the ExaTENSOR virtual processor is based on a hierarchical task-based parallel runtime built from scratch specifically for this project. This runtime can be extended to run on other HPC hardware architectures by providing node-level libraries which implement the necessary numerical tensor primitives for given hardware.