**Enabling Large-Scale GPU-Accelerated Correlated Quantum Chemistry Calculations: The Divide-Expand-Consolidate Scheme**
Dmytro Bykov, Ashleigh Barnes, and Dmitry Lyakh
Oak Ridge National Laboratory
barnesal@ornl.gov

**Abstract**

The divide-expand-consolidate (DEC) scheme can be applied to evaluate molecular energy and properties in a linear-scaling and embarrassingly parallel manner using a set of local Hartree-Fock molecular orbitals. The essence of the method lies in the fact that all manipulations with the intermediate four-dimensional quantities are carried out independently within small local orbital fragment spaces. The sizes of the orbital fragment spaces are determined in a black-box manner to ensure that the error in the DEC implementation is proportional to a single input threshold, denoted as the fragment optimization threshold (FOT). GPU-acceleration of the DEC scheme is achieved using both OpenACC was well as the TAL-SH library which allows for offloading of tensor contraction operations to GPUs. The scaling behavior, performance and benchmark studies as well as series of showcase calculations prove the DEC method to be a highly effective tool for approaching large molecular systems.