Massively Parallel Implementations of the Unrestricted Coupled Cluster Methods within Divide-Expand-Consolidate Scheme

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Often unique catalytic, spectroscopic and magnetic properties as well as chemical reactivity are direct consequence of the open-shell electronic structure. Nevertheless, implementations of unrestricted methods, capable of treating open-shell systems are less common than closed-shell. Here we present massively parallel implementation of coupled cluster (CC) methods based on our in-house developed chain of tools: equation generator, code generator and tensor computation library – ScaTeLib. The tool chain is tailored to the LSDalton program[1] and can be straightforwardly extended to work within the divide-expand-consolidate (DEC)[2] scheme. The DEC scheme is a local CC approximation which can be applied to evaluate CC energy and molecular properties in a linear-scaling and embarrassingly parallel manner.
The workflow includes generation of the tensor contractions from the commutator expressions and implementing them using simple unified interface of the ScaTeLib library. The library interface does not depend on the tensor storage type, number of modes or contraction patterns. The library enables storage of tensors in a dense format on a single computational node as well as in the parallel-distributed memory. The graphical processing units (GPU) support is also available. Thus, resulting implementations are linear-scaling, massively parallel and GPU ready.

ACKNOWLEDGMENTS: This research used resources of the Oak Ridge Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC05-00OR22725.

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