Automating Reduced-Scaling Many-body Methods With SeQuant: an Open-Source General-Purpose Symbolic Tensor Algebra System for Quantum Physics

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Recent emergence of reduced-scaling many-body methods based on block-rank-compressed forms of wave operator, such as pair natural orbitals-based coupled-cluster methods, allows accurate and routine many-body computations on systems with hundreds and thousands of atoms on a single HPC node. Unfortunately, such methods are technically complex due to the need to implement extensive (block-)sparse tensor algebra. Automated implementation techniques that have been demonstrated for conventional many-body methods are an attractive way to simplify the development of the reduced-scaling many-body methods. Here we demonstrate SeQuant, an open-source general-purpose symbolic tensor algebra system for quantum physics, that is capable of automated derivation, transformation, and evaluation of the tensor algebra for PNO-based and other related approaches to reduced scaling. SeQuant uses an efficient implementation of Wick's theorem to derive methods. The tensor expressions are canonicalized in presence of symmetries by leveraging colored graph canonization. The single-term optimization is efficiently performed by dynamic programming techniques. By integrating SeQuant with the TiledArray tensor framework it is now possible to obtain a distributed-memory parallel and, eventually, heterogeneous implementations of the reduced-scaling many-body methods.