Abstract

Firstly, we have developed a Tensor Contraction Engine-based implementation of the BW-MRCCSD approach. The scalability tests have been performed across thousand of cores. We have further developed a novel two-level parallel algorithm for Hilbert-space MRCC methods which uses the processor groups. In this approach, references are distributed among processor groups (reference-level parallelism) and tasks of each reference are distributed inside of a given processor group (task-level parallelism). We have shown that our implementation scales across 24000 cores. The usability of our code was demonstrated on larger systems (dodecane, polycarbenes and naphthyne isomers). Finally, we present novel universal state-selective (USS) corrections to the state-specific MRCC methods. The USS-corrected MRCC results were compared with the full configuration interaction (FCI) results.