Simulation of massively-parallel PNO-based CCSD(T) and EOM-CCSD

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Abstract:
Nearly all quantum chemical methods development research seeks to increase computational efficiency either by developing reduced-scaling methods or by implementing current methods in a more highly parallelized manner. A combination of these two tactics can, however, lead to more increases in efficiency than either one alone. This current work explores one such synthesis. We have simulated a pair natural orbital (PNO) based coupled cluster result within the highly parallel framework of the Massively Parallel Quantum Chemistry (MPQC) package [1]. The use of PNOs allows us to decrease the scaling of highly accurate methods while tightly controlling the error incurred The idea behind PNOs is simple: for each pair of occupied molecular orbitals, certain unoccupied molecular orbitals will contribute more substantially to the electronThese reduced-scaling methods can then be readily implemented in a highly-parallel manner using pair natural orbitals (PNOs) to decrease the scaling of certain highly accurate methods while carefully controlling the loss in accuracy that comes as a result

References

[1] Fabijan Pavosevic, Peter Pinski, Christoph Riplinger, Frank Neese, Edward F. Valeev, "SparseMaps - A systematic infrastructure for reduced-scaling electronic structure methods. IV. Linear-scaling second-order explicitly correlated energy with pair natural orbitals", J. Chem. Phys., **2016**, *144*, 144109

[2] "MPQC4: Massively Parallel Quantum Chemistry", Edward F. Valeev, Cannada A. Lewis, Chong Peng, Justus A. Calvin, Jinmei Zhang, `https://github.com/valeevgroup/mpqc4`.