POSTER ABSTRACT

Superlinear Parallel Scaling of Second Order Møller-Plesset Perturbation Theory on Modern High Performance Computation Clusters through the Employment of Quadrature Schemes

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Utilising the massively parallel, often heterogeneous, resources of modern high performance computation clusters for ab initio wave function-based methods is not straightforward. These methods typically have fundamental bottlenecks, e.g. they require basis set transformations of two electron integrals which involve a lot of data communication and have only bad parallelizability. This limits their scalability.

We followed the scheme behind the Q-MP2-OS formulation of Barca et al. [1], which involves independent evaluations of the recast energy integral through quadrature techniques.

Through this we arrived at a variant for the full Q-MP2 expression, which shows superlinear parallel scaling on modern high performance clusters. The independent evaluations allow for efficient exploitation of cache effects and minimal communication between nodes.

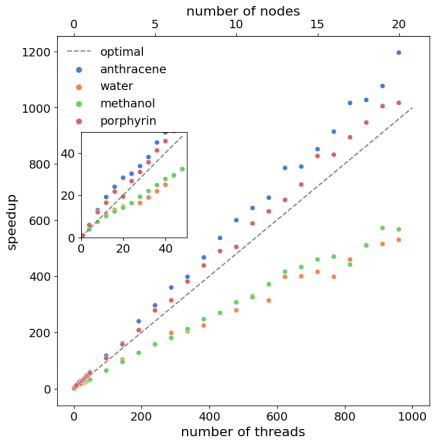

Figure 1 Parallel speedup of the Q-MP2 correlation energy calculation for a select number of trial systems on the JUSTUS 2 nodes with 2×24 physical cores per node.

References

[1] G.M. Barca, S.C. McKenzie, N.J. Bloomfield, A.T. Gilbert and P.M. Gill, Journal of Chemical Theory and Computation **16** (3), 1568–1577 (2020).

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