Q-MP2-OS: A new approach to correlation using quadrature

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As computational hardware becomes ever more massively parallel, quantum chemical methods and their underpinning implementations must evolve. In this lecture, I will present a novel algorithm [1] for the computation of the opposite-spin (OS) MP2 correlation energy, which is well suited to large-scale parallelization.

The method combines deterministic numerical quadratures and screening techniques, and entirely avoids the computation of any two-electron integrals. Speedup, scaling and accuracy results for a variety of molecules and reactions reveal that the new algorithm achieves 1 kcal/mol accuracy with almost perfect parallelizability (Fig. 1) and a computational cost which grows only quadratically with system size.

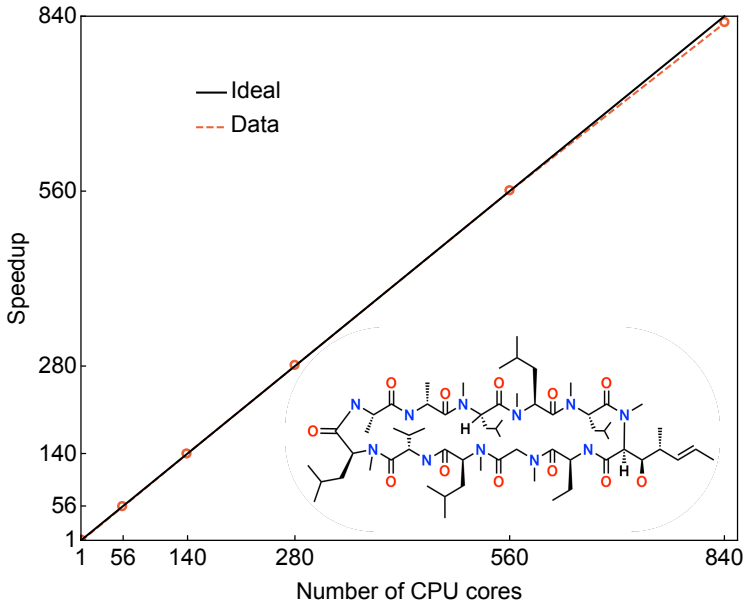

Figure 1: Speedup curve for Q-MP2-OS/6-31G on cyclosporine.*

References

1. GMJ Barca, SC McKenzie, NJ Bloomfield, ATB Gilbert and PMW Gill, submitted.