# High Performance and High Accuracy are Not Mutually Exclusive

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The coupled cluster family of methods provides a systematically improvable route to high accuracy in molecular calculations. Climbing this ladder of methods towards the exact solution incurs increases in the cost of the calculation, with e.g. CCSDTQ ($O(n^{10})$) being more expensive than CCSDT ($O(n^8)$), which in turn is more expensive than CCSD ($O(n^6)$), etc. However, even besides this largely unavoidable increase in asymptotic complexity of coupled cluster, these more highly accurate methods have traditionally suffered from much lower absolute computational efficiency (i.e. % of machine peak) as well as reduced parallel scalability. The loss of just this constant factor in efficiency has hampered application of these methods on a wide scale.

In this talk, we will explore several new theoretical and computational techniques relating to high accuracy coupled cluster methods, especially with regards to tensor contraction, which is the fundamental computational kernel of coupled cluster and other quantum chemical approaches. Additionally, we will show how adoption of modern computational techniques and software engineering practices has enabled a revolutionary simplification in the implementation of new high accuracy quantum chemistry methods.