Reduced Active Spaces and External Correlation

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Given the recent stagnation in CPU performance, it can be insightful to reconsider previously commonly-used methods to reduce the cost of correlation calculations. Specifically, this talk will cover ways of choosing subsets of orbitals to use in coupled-cluster calculations. This talk will also cover the related issue of how to account for the correlation effects arising from the excluded orbital spaces. A modern take on the old approaches to account for external correlation will be introduced, and the interplay between methods for choosing active orbital spaces and methods for accounting for the missing external correlation will be discussed.