Cholesky-Decomposed Densities in Laplace-Based Second-Order Møller-Plesset Perturbation Theory

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We present a modification of our linear-scaling AO-MP2 method [1-3] employing Cholesky-decomposed [4,5] pseudo-density (CDD) matrices [6]. This leads to an energy expression involving only fully transformed integrals (FTIs) over localized pseudo-MOs. Using an integral screening procedure based on rigorous Schwarz and MBIE upper bounds [1], the asymptotic scaling of the number of required FTIs is reduced to linear for non-delocalized systems. Due to the restriction of indices to the occupied and virtual subspaces, important performance gains are obtained as compared to standard AO-MP2, in particular for large basis sets. Results for both the pure CDD-MP2 algorithm as well as the corresponding approach employing the 'resolution of the identity' (RI) technique [6,7] for the formation of integrals are presented. In contrast to CDD-MP2, the RI-CDD-MP2 approach sacrifices the linear-scaling behavior in favor of a significant prefactor reduction, effectively leading to higher performance for medium-sized and even relatively large molecules.

Literature:

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