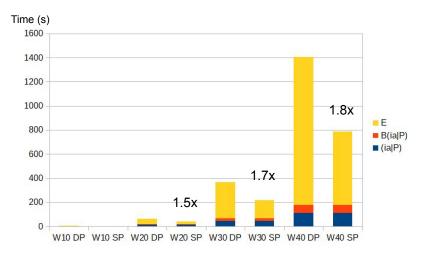


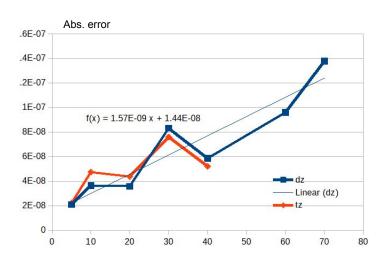
Evaluation of RI-MP2 correlation energy using mixed precision arithmetic

$$E = \sum_{ijab} \sum_{P} \frac{\left[B_{ia}^{P} B_{jb}^{P} - B_{ib}^{P} B_{ja}^{P} \right]^{2}}{(e_i + e_j) - (e_a + e_b)}$$

Computational speedup due to using single-precision MM for B*B contractions



Absolute error in final RI-MP2 energy due to reduced precision. Values below 10⁻⁶ are acceptable.



Problem size