Programming Project 6: MP2
Second-order Møller-Plesset perturbation theory (spin-orbital)

Let $\{\psi_p\}$ be canonical Hartree-Fock spin-orbitals with orbital energies $\{\epsilon_p\}$ and basis expansion coefficients $C_{\mu p}$.

$$\langle \psi_p \psi_q | \psi_r \psi_s \rangle = \sum_{\mu\nu\rho\sigma} C^*_{\mu p} C^*_{\nu q} C_{\rho r} C_{\sigma s} \langle \xi_\mu \xi_\nu | \xi_\rho \xi_\sigma \rangle \tag{1}$$

$$E^{(2)} = \frac{1}{4} \sum_{ijab} \frac{|\langle \psi_i \psi_j || \psi_a \psi_b \rangle|^2}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b} \tag{2}$$

Procedure

1. Run canonical spin-orbital Hartree-Fock code to obtain MO coefficients $\{C_{\mu p}\}$ and orbital energies $\{\epsilon_p\}$.
2. Transform two-electron integrals from the spin-AO basis $\{\xi_\mu\}$ to the spin-MO basis $\{\psi_p\}$ (equation 1)
3. Evaluate MP2 energy expression (equation 2)