

The one electron integrals are much more easy for me to conceptualize, but the two electron integrals are more tricky. The code for them that I have right now when there are no differences in the determinants is:

$(1/2)*\text{np.sum}(\text{two_elec_integrals}, (0,1))*(\text{two_elec_integrals}[0, 0, 1, 1]-\text{two_elec_integrals}[0, 1, 0, 1])$. In $\text{np.sum}(\text{two_elec_integrals}, (0,1))$, `two_elec_integrals` has `h2e.npy` loaded in, and the tuple `(0, 1)` means the summation is supposed to run over the first and second axes. `two_elec_integrals[0, 0, 1, 1]` is supposed to mean `[mm|nn]`, Where I am summing over the index `m` and `n` separately. I haven't tried out this code yet, but I realize that if I get the mathematics completely wrong, it will be nearly impossible to debug.