CS205 High-Level Project Description

February 2023

1 Moller-Plesset Correction to Hartree Fock Energies

- Parallelize the contraction of the electron repulsion integral from the atomic orbital basis to the molecular orbital basis. This should be possible through the use of pragma omp collapse(4) if we explicitly write out the tensor contraction. I am not sure if MPI is needed for this although depending on the size of the matrix it could be a good idea to allow multiple nodes.
- Parallelize the MP2 energy. This is once again going to be done using pragma omp collapse(4). Same considerations for MPI.
- We can parallelize the construction of one and two electron integral matrices. Both of these should be parallelize-able using a for loop construct by declaring each variable thread private (I may be misunderstanding threadprivate but the idea is construct each tensor separately then add them together at the end of the computation, each index is unique).