Hartree Fock Fortran Project

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1 TO DO

1. Install prerequisites

2 GOAL

We want to write a program that is able to perform Hartree-Fock calculations, both restricted and unrestricted. We also wish to have options for frozen core approximations. To perform the calculations we will use the TALSH library written by Lyakh. This will allow us to perform calculations on multiple nodes, however only one node will be used during the project (only home computer). Given are two tensors $\mathbf{h}^{core}$ and $\mathbf{g}$ and the tensors for the Fock and density matrices must be computed.

3 OPTIMISATIONS

Working in space of n orthogonal spinorbitals, so overlap matrix is unit matrix. We start with a diagonal density matrix for our trial matrix.

4 PROGRAM FLOW

4.1 Program Folder

– src
—— gp
——— qalgebra.f
—— main.f90
—— hf.f90
—— input
——— 001.in
——— 002.in
——— etc...

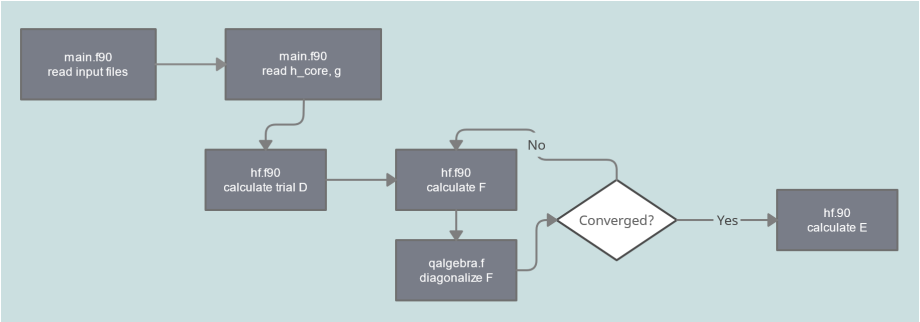

Figure 1: Program flow for the HF calculation.

4.2 main.f90

Main program which takes input files and initialises the required options and calculations. For the matrices we shall use double precision complex typed arrays of size 2n. It may be smart to define a new type for the spinorbitals consisting of exponential factors and centres of the basis function (assuming Gaussian basis). We also must read or calculate the core Hamiltonian and 2-electron integral matrices.

4.3 hf.f90

Module implementing the procedures for calculating the Hartree-Fock and density matrices and other objects. Again, matrices are implemented as complex double precision arrays. We need a number of subroutines. One for calculating the various matrices, including the density and Fock matrices. We also need a subroutine or function to calculate the energy, for which we need to use the core Hamiltonian and 2-electron integrals. Finally we need a subroutine to perform the SCF iterations, for which we use the Fock-matrix subroutine.

4.4 input

Folder containing input files. We can use a json-style file type to simplify the settings. We want to include options for number of electrons, number of basis functions, whether to use restricted or unrestricted HF, whether to use frozen core and which functions to use.