Hartree-Fock Implementation for Pedagogical & Research Purposes

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Gary Zeri, Jerry LaRue

Computational Chemistry is the use of computers and quantum mechanics to simulate chemical experiments, saving time and money for scientists and researchers. Despite the benefits of computational chemistry, few undergraduate students are exposed to computational chemistry methods. Because of this, there is a need for an easily understandable computational-chemistry code with a focus on pedagogical use, leading to the implementation of the Hartree-Fock method in Python, with a focus on legibility and conceptual understanding for undergraduate students. The overall logic flow of the program is depicted below.

**Specify Molecular System**
- Atomic Numbers
- Nuclear Coordinates
- Number of Electrons
- Basis Set
- Object-Oriented Structure (Atoms build Molecules)

**Evaluate Integrals**
- Gaussian Basis Set allows for simplification of integral evaluation
- Evaluate integrals for overlap, electron kinetic energy, electron repulsion, and nuclear-electron attraction values

**Prepare for SCF**
- Construct Hamiltonian
- Construct Guess Fock Matrix, Assume no Electron-Electron Interactions for Guess
- Create Transformation Matrix

**SCF Procedure**
- Compute molecular orbitals and energies from transformed Fock matrix

**Diagonalize Fock Matrix**
- Use molecular orbitals to compute density of electrons

**Build Density Matrix**
- Use density matrix to build two electron term

**Build Two Electron Term**
- Use two electron term and Hamiltonian to create a new Fock matrix

**Rebuild Fock Matrix**
- Determine energy of the molecule from the Fock matrix

**Compute Expectation Energy**
- Check if difference between expectation energies is less than a certain threshold

**Check For Convergence**
- Convergence Reached
- Output Computed Energy & Bond Distance

**Convergence No Reached**
- Pedagogical SCF Method

**Simulated Results**
Graph of hydrogen atom ground state energies at varying bond lengths. Data was generated from pedagogical Hartree-Fock code.

**References**